VOLUME II

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We also would like to thank the plenary speakers and the plenary panel speakers: Gerald Boyd, the Deputy Assistant Secretary for the Department of Energy's Office of Science and Technology (DOE/OST); Tom Baca, Program Director, Environmental Management Division, Los Alamos National Laboratory; David McWhorter, Professor of Chemical and Bioresource Engineering, Colorado State University; David Bluck, Simulation Sciences Inc.; Caroline Purdy (DOE/OST); Subhas Sikdar (EPA); Lester Lave (Carnegie Mellon University); Alan Pritsker (Pritsker Corporation); and Jeffrey Holland (DoD).

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Appendix A. List of Attendees and Interest Area Team Members

A.1 List of Attendees

Name	Organization	Phone	Interest Area Team
Adams, Andrew	Los Alamos National Laboratory	505-667-0959	Actinides
Aleman, Sebastian	Westinghouse Savannah River Co.	803-725-8205	Subsurface Contamination II
Allen, George	Sandia National Laboratories	505-844-9769	Subsurface Contamination II
Aloyan, Artash	INM RAS Inst. of Math., Russia	7-095-938-3767	Environmental Security
Ashwood, Tom	Oak Ridge National Laboratory	423-574-7542	Health and Ecological Effects II
Atkinson, Peter W.	ALIAS Group, Incorporated	703-941-2485	Environmental Security
Avramenko, Mikhail I.	Russian Federal Nuclear Center-VNIITF	7-351-72-32930	Environmental Security
Baca, Tom	Los Alamos National Laboratory	505-667-2211	Speaker
Baker, Jim	Michigan Tech. University	906-487-3143	Manufacturing/Pollution Prevention
Barr, Sumner	Los Alamos National Laboratory	505-667-3203	Environmental Security
Benze, Robert	U.S. Navy	360-476-8448	Health and Ecological Effects I
Berger, Michael	Los Alamos National Laboratory	505-667-2211	Infrastructure
Birdsell, Kay	Los Alamos National Laboratory	505-665-0260	Organizing Committee; Subsurface Contamination I, Reporter
Bluck, David	Simulation Sciences Inc.	714-985-5235	Speaker; Manufacturing/Pollution Prevention
Boak, Jeremy	Los Alamos National Laboratory	505-667-0835	Organizing Committee; Manufacturing/Pollution Prevention, Reporter
Booth, Steven	Los Alamos National Laboratory	505-667-9422	Infrastructure
Boyd, Gerald	DOE/EM Office of Science and Technology	202-586-6382	Executive Committee; speaker
Brusuelas, Richard	County of Bernalillo	505-924-3650	Health and Ecological Effects I
Burford, Tom	DOE/AL	505-845-9893	
Bushong, Phil	Naval Surface Warfare Center	540-653-4782	Health and Ecological Effects I
Butner, Scott	Pacific Northwest National Laboratory	206-528-3290	Manufacturing/Pollution Prevention, Chair
Cabezas, Heriberto	EPA National Risk Management Research Laboratory	513-569-7350	Executive Committee; Manufacturing/Pollution Prevention

Name	Organization	Phone	Interest Area Team
Cahn, Lorie	Waste Management Federal Services	208-526-4283	
Cary, Steve	DoD/ODUSD (ES)	703-697-7363	Executive Committee
Chacon, Michael	NMED - Haz & Rad	505-827-1558	
Chen, S.Y.	Argonne National Laboratory	630-252-7695	Decontamination and Decommissioning
Chromec, Win	Rocky Mountain Remediation Services	303-966-4535	Health and Ecological Effects I
Clark, Frances	Argonne National Laboratory	630-252-1180	Decontamination and Decommissioning
Cline, Patricia	CH2M HILL	352-335-7991	Subsurface Contamination I
Cofalka, Piotr	IETU Katowice, POLAND	48-32-2546031	Environmental Security
Corey, John C.	WSRC - SRTC	803-725-1134	Subsurface Contamination II
Cormier, John	DOE	505-845-5956	Manufacturing/Pollution Prevention
Cornils, Kristine	ICF Kaiser	202-863-7031	Waste Treatment
Daily, Christine	U.S. Nuclear Regulatory Commission	301-415-6026	Decontamination and Decommissioning
Davidson, Joseph	Phillips Petroleum Co.	918-661-4054	Subsurface Contamination I
Davis, Teri	NMED - Haz & Rad	505-827-1558	
de la Cruz, Vanessa	Los Alamos National Laboratory	505-667-5648	Organizing Committee
Ditmars, Dr. John D. (Jack)	Argonne National Laboratory	630-252-5953	Environmental Security
Diwekar, Urmila	Carnegie Mellon University	412-268-3003	Manufacturing/Pollution Prevention
Dixon, David	Pacific Northwest National Laboratory	509-372-4999	Actinides
Dorries, Alison	Los Alamos National Laboratory	505-665-4791	Health and Ecological Effects II
Doss, Said K.	Lawrence Livermore National Laboratory	510-423-4281	Subsurface Contamination I
Douglas, Karen	US Department of Energy	505-845-6411	Subsurface Contamination II
Dunning, Donald	Argonne National Laboratory	423-576-5730	
Duvall, Ken	DOE Office of Environmental Policy	202-586-0242	Decontamination and Decommissioning
Ebinger, Michael	Los Alamos National Laboratory	505-667-3147	Organizing Committee; Health and Ecological Effects II, Reporter
Economy, Kathy M.	Sandia National Laboratories	505-766-9629	Subsurface Contamination I
Erdal, Bruce R.	Los Alamos National Laboratory	505-667-5338	Executive Committee; Decontamination and Decommissioning

Name	Organization	Phone	Interest Area Team
Esh, David	Argonne National Laboratory-West	208-533-7100	Actinides
Evans, Susan	LIMITCO	208-526-1493	
Faybishenko, Boris	Lawrence Berkeley National Laboratory	510-486-4852	Subsurface Contamination I
Featherman, David	Project Performance Corporation	617-524-3196	Decontamination and Decommissioning
Ferenbaugh, Roger W.	Los Alamos National Laboratory	505-667-0811	Organizing Committee; Health and Ecological Effects I, Reporter
Ferryman, Tom	Pacific Northwest National Laboratory	509-375-3888	Infrastructure
Finley, Virginia	Princeton Plasma Physics Laboratory	609-243-2746	Health and Ecological Effects II
Foley, Michael	Pacific Northwest National Laboratory	509-372-4671	Subsurface Contamination I
Fravel-Meyers, Jeanne	Naval Surface Warfare Center, Dahlgren Division	540-653-4780	Health and Ecological Effects II, Chair
Freer, Jerry E.	Los Alamos National Laboratory	505-665-7023	Waste Treatment, Reporter
Ghassemi, Abbas	WERC	505-646-7697	Waste Treatment, Chair
Gibbs, Bruce	Fusion And Control Technology, Inc. (FACT)	301-474-4541	Subsurface Contamination I
Glagolev, Dr. Andrei	PSA Hydrospetzgeologiya, Russia	095-150-5759	Subsurface Contamination I
Gonzales, Johnell	Los Alamos National Laboratory	505-667-8110	Manufacturing/Pollution Prevention
Gordon, Joe	MACTEC	303-494-8997	Health and Ecological Effects II
Greene, Robert K.	Los Alamos National Laboratory	505-665-0340	Environmental Security
Hannon, W. Jim	Lawrence Livermore National Laboratory	510-422-6452	Environmental Security, Chair
Hansen, Wayne	Los Alamos National Laboratory	505-667-3331	Health and Ecological Effects I
Hanson, Steve	Los Alamos National Laboratory	505-667-4301	
Hardie, R. Wayne	Los Alamos National Laboratory	505-667-2442	Infrastructure, Chair
Harper, Johnny	Los Alamos National Laboratory	505-665-6156	Organizing Committee; Decontamination and Decommissioning, Reporter
Harris, Mary	Westinghouse Savannah River Co.	803-725-4184	Subsurface Contamination I
Hart, Paul	US Department of Energy	304-285-4358	Decontamination and Decommissioning, Chair

Name	Organization	Phone	Interest Area Team
Hassman, B.J	Los Alamos National Laboratory	505-667-4301	Waste Treatment
Hertel, William	Fluor Daniel Fernald	513-648-3894	Subsurface Contamination II
Hill, Kim	HMED - Haz & Rad	505-827-1558	
Hirshberg, Susan	The Sanctuary Foundation	505-988-2939	Health and Ecological Effects II
Hjeresen, Dennis	Los Alamos National Laboratory	505-665-7251	Organizing Committee; Environmental Security, Reporter
Hlohowskyj, Ihor	Argonne National Laboratory	630-252-3478	Health and Ecological Effects I
Ho, Cliff	Sandia National Labs		Subsurface Contamination II
Hoberg, Alan	Battelle	614-424-5706	Subsurface Contamination I
Holland, Jeffery	Department of Defense	601-634-2644	Panelist; Subsurface Contamination II, Chair
Hollis, Diana	UC/LANL	505-665-8469	Actinides
Huyakorn, Peter	HydroGeoLogic, Inc.	703-478-5186	Subsurface Contamination II
Jacobson, Jacob J.	Lockheed Martin Idaho	208-526-3071	Environmental Security
Janecky, David	Los Alamos National Laboratory	505-665-0253	Organizing Committee; Actinides, Reporter
Jensen, Reed	Los Alamos National Laboratory	505-667-2211	Environmental Security
Johnson, Tod	University of Nevada, Las Vegas	702-895-4190	Subsurface Contamination II
Kendall, Richard	Los Alamos National Laboratory		
Ketelle, Richard	Oak Ridge National Laboratory	423-574-5762	Actinides
Kieling, John	NMED - Haz & Rad	505-827-1558	
Kirchner, Tom	New Mexico State University	505-234-5504	Health and Ecological Effects I, Chair
Kjeldgaard, Ed	Sandia National Laboratories	505-845-8011	Manufacturing/Pollution Prevention
Knowlton, Robert	DecisionFX, Inc.	505-869-0057	Health and Ecological Effects II
Krahl, David	Imagine That, Inc.	408-365-0305	Manufacturing/Pollution Prevention
Krummel, John	Argonne National Laboratory	630-252-7648	Health and Ecological Effects I, Chair
Kurochkin, Vitaliy M.	Institute of Production Engineering, Russia	095-3245196	Subsurface Contamination I
Kwok, Kwan S.	Sandia National Laboratories	505-845-7170	
Laase, Alan	Oak Ridge National Laboratory	970-248-6250	Actinides
Lave, Lester	GSIA Carnegie Mellon University	412-268-8837	Panelist; Manufacturing/ Pollution Prevention

Name	Organization	Phone	Interest Area Team
Lee, H. N. (Sam)	Environmental Measurements Lab.	212-620-6607	Manufacturing/Pollution Prevention
Lewis, Johnnye L.	Environmental Health Associates	505-469-3028	Health and Ecological Effects I
Li, Bai-Lian (Larry)	The University of New Mexico	505-277-5140	Health and Ecological Effects I
Li, Zhe	CAEP, China	86-816-2486722	Environmental Security
Liang, Shuquing	CAEP, China	86-10-62014411	Environmental Security
Little, Craig	Oak Ridge National Laboratory (Life Sciences)	970-248-6201	Environmental Security
Liu, Ning	SAIC	702-295-5072	Decontamination and Decommissioning
Lober, Bob	DOE-RL	509-373-7949	Subsurface Contamination I
Longmire, Patrick	Los Alamos National Laboratory	505-665-1264	Subsurface Contamination II
Maccabe, Andrew	Armstrong Lab/Health Risk	210-536-6113	
Malinauskas, A.P.	Oak Ridge National Laboratory	423-576-1092	Waste Treatment
Maltese, Jay G.	Halliburton Mus. Corporation	301-258-5820	Health and Ecological Effects I
Marchetti, John A.	DOE Defense Programs	301-903-3487	Executive Committee; Manufacturing/Pollution Prevention, Chair
Martin, Beverly	Los Alamos National Laboratory	505-665-7430	Health and Ecological Effects II
Martinez, Mario	Sandia National Laboratories	505-844-8729	Subsurface Contamination I
May, Ira	US Army Environmental Center	410-671-1522	Subsurface Contamination I
McGuire, Stephen	U. S. Nuclear Regulatory Commission	301-415-6204	Subsurface Contamination I
McLaughlin, Peter	Battelle	253-512-2212	Waste Treatment
McPherson, Elizabeth	McPherson Envir. Res.	423-543-5422	Manufacturing/Pollution Prevention
McWhorter, David	Colorado State University	970-491-8666	Executive Committee; Speaker; Subsurface Contamination I, Chair
Mikhalevich, Alexander A.	Institute of Power Engineering Problems, Russia	375-172-260698	Actinides
Miller, Ian	Golder Associates Inc.	425-883-0777	Subsurface Contamination I
Miller, W. Lamar	University of Florida	352-392-7101	Executive Committee; Organizing Committee; Waste Treatment, Chair, Reporter
Myers, Jonathan	IT Corporation	505-262-8726	Actinides
Norris, Tom	Los Alamos National Laboratory	505-667-1136	Actinides
Oldenburg, Curtis	Lawrence Berkeley National Laboratory	510-486-7419	Health and Ecological Effects I

Name	Organization	Phone	Interest Area Team
Oudejans, Miriam	Los Alamos National Laboratory/LATA	505-667-4028	Organizing Committee
Parnell, Gregory S.	Virginia Commonwealth University	804-828-1301	Subsurface Contamination I
Peake, Tom	U.S. Environmental Protection Agency	202-233-9765	Actinides
Pendergrass, John H.	Los Alamos National Laboratory	505-667-2266	Organizing Committee; Infrastructure, Reporter
Persichetti, John	Horizon Technologies	303-972-2530	Manufacturing/Pollution Prevention
Peterson, Suzanne	Los Alamos National Laboratory	505-665-6712	
Petullo, Colleen F.	US EPA/ORIA-RIENL	702-798-2446	Decontamination and Decommissioning
Phelan, James	Sandia National Laboratories	505-845-9892	
Piskunov, Vladimir	VNIIEF Arzamas 16 (Sarov), Russia	83130-45778	Environmental Security
Pohl, Phillip	Sandia National Laboratories	505-844-2992	
Pollock, David	U.S. Geological Survey	703-648-5007	Subsurface Contamination II
Pratt, Allyn	Los Alamos National Laboratory	505-667-4308	Health and Ecological Effects I
Price, Belinda	IT Corporation	423-690-3211	Subsurface Contamination I
Pritsker, A. Alan	Pritsker Corp.		Executive Committee; panelist; Infrastructure
Pruess, Karsten	Lawrence Berkeley National Laboratory	510-486-6732	Subsurface Contamination I, Chair
Purdy, Caroline	DOE/EM Office of Science and Technology	301-903-7672	Executive Committee; panelist; Infrastructure
Ramsey, Beverly	ATL	301-515-7679	Actinides, Chair
Regens, James	Tulane University Medical Center	504-586-3824	
Rehfeldt, Ken	DOE/NV	702-295-2503	Subsurface Contamination I
Reiser, Anita	Sandia National Laboratories	505-848-0131	Waste Treatment
Reuter, Stephen	New Mexico Environment Department	505-827-2566	Subsurface Contamination II
Richards, Dave	US Army Waterways Expt. Station	601-634-2136	Subsurface Contamination II
Robershotte, Mark	Battelle, PNNL	509-376-5627	
Roberts, Randy	Intera, Inc.		Decontamination and Decommissioning
Rogers, Phil	Jacobs Engineering Group	509-943-9297	Subsurface Contamination I
Romanovski, Vadim	Lawrence Livermore National Laboratory	510-423-9044	Actinides

Name	Organization	Phone	Interest Area Team
Romanovski, Valeri N.	V.G. Khlopin Radium Institute, Russia	812-247-65-22	Waste Treatment
Rosenberg, Nina	Los Alamos National Laboratory	408-459-5858	Subsurface Contamination I
Ross, Timothy	University of New Mexico	404-892-3099	Health and Ecological Effects I
Ryti, Randall	Neptune and Company, Inc.	505-665-2121	Health and Ecological Effects I
Rzeszotarski, Peter	US Army Envir. Policy Inst.	404-892-3099	
Savignac, Noel	Noel Savignac Consultants	505-881-4150	Health and Ecological Effects I
Schram, Susan	Consortium for International Earth Science Information Network	202-775-6611	Infrastructure
Schwinkendorf, William	LMITCO (c/o Sandia National Laboratories)	505-284-3993	Waste Treatment
Shafer, David	US Department of Energy	509-376-9255	Subsurface Contamination II
Shaner, Marja	Los Alamos National Laboratory	505-665-7112	Executive Committee
Shropshire, David	Lockheed Martin Idaho Technologies	208-526-6800	Waste Treatment
Sikdar, Subhas	EPA National Risk Management Research Laboratory	513-569-7528	Panelist; Manufacturing/ Pollution Prevention
Smoot, John	Pacific Northwest National Laboratory	509-372-6064	
Snyder, Kenneth	DOE	303-275-4819	
Springer, Everett	Los Alamos National Laboratory	505-667-3331	Environmental Security, Chair
Sullivan, Terry	Brookhaven National Laboratory	516-344-2840	Infrastructure
Swift, Peter	Sandia National Laboratories	505-848-0699	Actinides
Taffet, Michael	Lawrence Livermore National Laboratory	510-422-6114	Subsurface Contamination II
Tappen, Jeff	SAIC	702-295-5027	Health and Ecological Effects II
Temkar, Prakash	Army Environmental Policy Institute	404-892-3099	Environmental Security
Thron Jr., Harry M.	DOE/EM Office of Environmental Restoration		Executive Committee
Torak, Lynn	U.S. Geological Survey	770-903-9100	Health and Ecological Effects II
Toth, Barbara	NMED	505-827-1558	Health and Ecological Effects II
Tracy, John C.	Desert Research Institute	702-673-7385	Health and Ecological Effects I
Travis, Bryan	Los Alamos National Laboratory	505-667-1254	Organizing Committee; Subsurface Contamination II, Reporter
Unal, Cetin	Los Alamos National Laboratory	505-665-2539	Waste Treatment

Name	Organization	Phone	Interest Area Team
Valentine, Greg	Los Alamos National Laboratory	505-665-0299	Executive Committee; Organizing Committee
Van Eeckhout, Ed	Los Alamos National Laboratory	505-667-1916	Executive Committee; Organizing Committee
Vasil'kova, Nelly	PSA Hydrospetzgeologiya, Russia	095-251-4977	Subsurface Contamination I
Vaughn, Palmer	Sandia National Laboratories	505-848-0678	Subsurface Contamination I
Vopalka, Dusan	Czech Technical University, Czech Republic		Actinides
Wallace, William	Consortium for International Earth Science Information Network	970-490-8380	Infrastructure
Walter, Gary	Hydro Geo Chem, Inc.	520-623-6981	
Wang, Yifeng	Sandia National Laboratories	505-844-8271	Actinides
Webb, Stephen	Sandia National Laboratories	505-848-0623	Subsurface Contamination II
Weinrach, Jeffrey	Benchmark Environmental Corporation	505-262-2694	Manufacturing/Pollution Prevention
Wheelis, W.T. (Ted)	Sandia National Laboratories		Manufacturing/Pollution Prevention
White, Mark	Pacific Northwest National Laboratory	509-372-6070	Subsurface Contamination I
White, Ron	Fluor Daniel Fernald	513-648-5920	Subsurface Contamination II
Williams, Gus	Argonne National Laboratory	630-252-4609	Subsurface Contamination II
Williams, Joel D.	Los Alamos National Laboratory	505-667-9113	Actinides, Chair
Wolfinger, Thomas	DynaCorp	703-830-5945	Health and Ecological Effects II
Worland, Pete	Los Alamos National Laboratory	505-667-4301	Subsurface Contamination II
Yabusaki, Steven	Pacific Northwest National Laboratory	509-372-6095	Subsurface Contamination II, Chair
Young, John	NMED	505-827-1558	Subsurface Contamination II
Young, John	The Hampshire Research Institute	703-683-6695	Health and Ecological Effects II, Chair
Young, Steve	Roy F. Weston, Inc.		
Zenkowich, Mathew	DOE/EM Office of Waste Management	301-903-7126	Executive Committee; Waste Treatment
Zimmerman, D.A. (Tony)	Gram Inc.	505-299-1282	Subsurface Contamination II
Zinina, Galina	Institute of Physics and Power, Russia	08439-3-37-82	Subsurface Contamination I
Zlatev, Zahari	Natl. Environ. Res. Institute, Denmark	45-4630-1149	Environmental Security
Zou, Lexi	CAEP, China	86-816-2484204	Environmental Security

A.2 Interest Area Team Members

Actinides

Ramsey, Beverly—Chair
Williams, Joel D.—Chair
Janecky, David—Reporter
Adams, Andrew
Dixon, David
Esh, David
Hollis, Diana
Ketelle, Richard
Laase, Alan
Mikhalevich, Alexander A.
Myers, Jonathan
Norris, Tom
Peake, Tom
Romanovski, Vadim
Swift, Peter
Vopalka, Dusan
Wang, Yifeng

Decontamination and Decommissioning

Hart, Paul—Chair
Harper, Johnny—Reporter
Chen, S.Y.
Clark, Frances
Daily, Christine
Duvall, Ken
Erdal, Bruce R.
Featherman, David
Liu, Ning
Petullo, Colleen F.
Roberts, Randy

Environmental Security

Hannon, W. Jim—Chair
Springer, Everett—Chair
Hjeresen, Dennis—Reporter
Aloyan, Artash
Atkinson, Peter W.
Avramenko, Mikhail I.
Barr, Sumner
Cofalka, Piotr
Ditmars, Dr. John D. (Jack)
Greene, Robert K.
Jacobson, Jacob J.
Jensen, Reed
Li, Zhe
Liang, Shuquing
Little, Craig
Piskunov, Vladimir
Temkar, Prakash
Zlatev, Zahari
Zou, Lexi

Health and Ecological Effects I

Kirchner, Tom—Chair
Krummel, John—Chair
Ferenbaugh, Roger W.—Reporter
Benze, Robert
Brusuelas, Richard
Bushong, Phil
Chromec, Win
Hansen, Wayne
Hlohowskyj, Ihor
Lewis, Johnnye L.
Li, Bai-Lian (Larry)
Maltese, Jay G.
Oldenburg, Curtis
Pratt, Allyn
Ross, Timothy
Ryti, Randall
Savignac, Noel
Tracy, John C.

Health and Ecological Effects II

Fravel-Meyers, Jeanne—Chair
Young, John—Chair
Ebinger, Michael—Reporter
Ashwood, Tom
Dorries, Alison
Finley, Virginia
Gordon, Joe
Hirshberg, Susan
Knowlton, Robert
Martin, Beverly
Tappen, Jeff
Torak, Lynn
Toth, Barbara
Wolfinger, Thomas

Infrastructure

Hardie, R. Wayne—Chair
Pendergrass, John H.—Reporter
Berger, Michael
Booth, Steven
Ferryman, Thomas
Pritsker, A. Alan
Purdy, Caroline
Schram, Susan
Sullivan, Terry
Wallace, William

Manufacturing/Pollution Prevention

Butner, Scott—Chair
Marchetti, John A.—Chair
Boak, Jeremy—Reporter
Baker, Jim
Bluck, David
Cabezas, Heriberto
Cormier, John
Diwekar, Urmila
Gonzales, Johnell
Kjeldgaard, Ed
Krahl, David
Lave, Lester
Lee, H. N. (Sam)
McPherson, Elizabeth
Persichetti, John
Sikdar, Subhas
Weinrach, Jeffrey
Wheelis, W.T. (Ted)

Subsurface Contamination I

McWhorter, David—Chair
Pruess, Karsten—Chair
Birdsell, Kay—Reporter
Cline, Patricia
Davidson, Joseph
Doss, Said K.
Economy, Kathy M.
Faybishenko, Boris
Foley, Michael
Gibbs, Bruce
Glagolev, Dr. Andrei
Harris, Mary
Hoberg, Alan
Kurochkin, Vitaliy M.
Lober, Bob
Martinez, Mario
May, Ira
McGuire, Stephen
Miller, Ian
Parnell, Gregory S.
Price, Belinda
Rehfeldt, Ken
Rogers, Phil
Rosenberg, Nina
Vasil'kova, Nelly
Vaughn, Palmer
White, Mark
Zinina, Galina

Subsurface Contamination II

Holland, Jeffery—Chair
Yabusaki, Steven—Chair
Travis, Bryan—Reporter
Aleman, Sebastian
Allen, George
Corey, John C.
Douglas, Karen
Hertel, William
Ho, Cliff
Huyakorn, Peter
Johnson, Tod
Longmire, Patrick
Pollock, David
Reuter, Stephen
Richards, Dave
Shafer, David
Taffet, Michael
Webb, Stephen
White, Ron
Williams, Gus
Worland, Pete
Young, John
Zimmerman, D.A. (Tony)

Waste Treatment

Miller, W. Lamar—Chair, Reporter
Ghassemi, Abbas—Chair
Freer, Jerry E.—Reporter
Cornils, Kristine
Hassman, B.J
Malinauskas, A.P.
McLaughlin, Peter
Reiser, Anita
Romanovski, Valeri N.
Schwinkendorf, William
Shropshire, David
Unal, Cetin
Zenkowich, Mathew

Appendix B. Plenary Session Summary

The plenary session held on Day 1 set the stage for the ongoing theme of the workshop: reaching consensus on the most effective use of modeling in the DOE Environmental Management arena; explaining that use and providing decision makers and stakeholders with information in the format they need; and keeping in mind the three conditions under which modelers have to operate: budget, operational, and decision making.

Tom Baca, Program Director for Environmental Management at Los Alamos National Laboratory, opened the workshop with a welcome address that asked the participants to reach consensus on a rationale for the application of modeling and simulation to environmental problems. This rationale must be articulated in a manner that is useful for Congress and the public.

Gerald Boyd, the Deputy Assistant Secretary for DOE/Office of Science and Technology, went into more detail about the scope of the workshop, the constraints within which participants had to work, and challenges from a DOE/EM perspective. Acknowledging that a modeling and simulation capability already exists, Boyd defined the scope of the workshop as bringing these capabilities to bear on the right problems. Boyd emphasized the following three conditions:

(1) ***Budget***. The emphasis on modeling and simulation must have a broad focus. The workshop is not a call for proposals or new programs. This is not a new initiative. Modelers cannot start from scratch. The best strategy is to use information and results from previous uses of modeling and simulation. Boyd said we are operating within a “zero sum game,” which may worsen depending on the national economy over the next several years.

(2) ***Operational***. The DOE/EM planning process that will accelerate clean-up through 2006 is a major step forward. $60B will be spent in this process. In searching for a better, more cost-effective way to do this cleanup, field offices have been tasked with finding $8B in “efficiencies.” At the same time, these offices must continue to minimize risk to workers and the surroundings and face strong public scrutiny. Modelers need to plan downstream and show real payoffs. In order to reach the $8B efficiency target between now and 2006, modelers need better technology. They also need to recognize that the focus is on decision making and that stakeholders will continue their scrutiny. Worker and environmental safety is crucial—lack of a budget is no excuse for shortcomings in this area.

(3) ***Decision Making***. According to Boyd, we are not close to having optimal decision-making tools, but we have made progress. Alternative decision and technology tools are needed. Boyd offered the following challenges to the workshop: help DOE apply existing modeling and simulation techniques, look for overlaps and opportunities for further integration across environmental disciplines, and seek new, cost-effective techniques for further development. Effective communication with decision makers is essential. Modelers and decision makers need to work together more closely and share a common language in order to come to a consensus about prioritizing models and what needs to be modeled.

David McWhorter, Professor of Chemical and Bioresource Engineering, Colorado State University, gave a plenary talk that addressed some of the fundamental issues of modeling: the value of models, the process involved in creating models, some aspects of problem solving, and uncertainty. McWhorter defined *modeling* as the act of creating or using models and defined *models* as being mental, physical, or mathematical constructs that simulate some aspect of nature. Models can range from the conceptual to the quantitative.

The Value of Models

McWhorter said that the value of models depends on the purpose for which they are developed and used, and on particular requirements at a given time. The comparison of models of intrinsic value to direct use is at the core of science. The most visible and useful manifestation of science provides a connection among scientific observations.

Conceptual models perform a similar service, which is the construction of hypotheses and the subsequent manifestation of those hypotheses. Modelers must force a consistency among input and output variables. Functions and parameters enforce structure, which produces understanding by the resolution of models with field data. The value of models is connected to their objectives, but there are three basic major values: (1) models serve to organize facts, (2) they allow us to generalize our knowledge, and (3) they aid in the discovery of new knowledge.

Creating a Model

According to McWhorter, there are five major steps in creating a model:

1. Establish the objectives of the model.
2. Develop an appropriate conceptual model and scale of interest.
3. Synthesize information into a mathematical component or statement. This involves idealization and abstraction, both of which depend on the objectives.
4. Develop mathematical equations to solve the problem.
5. Confirm (verify and validate) the model.

Aspects of Problem Solving

McWhorter spoke about several aspects of problem solving:

- ***Forecasting or Prediction.*** History can sometimes calibrate the usefulness of the model (e.g., contaminant release, natural attenuation, threat to ground water from vadose zone) before forecasting is undertaken.
- ***Hindcasting.*** Hindcasting assigns responsibility by answering the following questions: What caused this contamination? How long will the effects of the exposure last?

Forecasting long-range effects is a bigger challenge than forecasting initial conditions and is more important for this analysis.

- ***Performance Analysis and Design.*** There is great growth potential in this area, particularly in remediation design. Source zone remediation is behind in development; it is currently being implemented without a knowledge of the likely effects (e.g., a multi-phase fluid flow in a heterogeneous environment).

Uncertainty

There is uncertainty associated with every model application, according to McWhorter. A major problem is the correct representation of uncertainty in models and the effective communication of that uncertainty to end users and decision makers. Reliability can be enhanced by mimicking available data. Models are indispensable in spite of flaws; enthusiasm should not obscure flaws.

Following McWhorter’s talk, David Bluck, from Simulation Sciences Incorporated, spoke on modeling in the chemical process industry. This industry uses modeling in the following areas:

- Planning—scheduling, planning, enterprise models
- Conversion of raw materials—flow simulation, optimization, network optimization, materials selection
- Raw materials process—design and retrofit, simulation and optimization
- Intermediate—debottlenecking, process improvement

The chemical industry strives to meet objectives of the corporate environment by defining “valve” positions, incorporating information on internal and external inputs, and by producing outputs. Chemical industry objectives take into account that the market forces long-range planning (internal information) 5 to 10 years down the road. This industry incorporates enterprise and equipment planning as well as coarse grained decision support using “linear program” tools. Short-term planning includes information culled from one month to one year.

Panel Discussions

Following the individual presentations, a panel discussion addressed modeling and simulation from a variety of perspectives including industry, DoD environmental programs, academia, DOE/EM, and EPA.

Industry. Alan Pritsker, CEO, the Pritsker Corporation, discussed the goals of industry: stay in business, increase worth, make a profit, and be a good corporate citizen. Most of these goals are economic, with the exception of “good citizenship,” which can have an environmental flavor. The type of environmental modeling and simulation that industry wants is that which is easy to use, reusable, off-the-shelf, monitor-and-control oriented, and embedded within the system at hand. As noted in the table below, fundamental differences between the “operating parameters” of a businessman and an environmentalist exist that are a source of conflict. The results of modeling and simulation need to be translated to capture the best elements of these competing factors.

Businessman	Environmentalist
short-time horizon	long-time horizon
quick decisions	decisions by hearings
economic goals with environmental constraints	environmental goals with economic constraints
control—job security	controls—regulations, legislative, and fiscal incentives

DoD Environmental Programs. Jeffrey Holland, DoD EQM Computational Technology Area Leader, provided some examples of success stories for modeling in the DoD's environmental work, such as the Schofield Army Barracks project where $5M was saved by judicious use of modeling approaches. Holland noted that the state of the art in environmental modeling and simulation is not generally used in actual cleanup problems. Holland cited four reasons why state-of-the-art models are not adopted:

(1) The most recent developments in modeling and simulation are not keyed to field problems and business practices.

(2) A lack of technical agreement on certain processes limits the transition of new research into practice.

(3) Users have a fear of embarking on a new learning curve because of the time and effort lost.

(4) A fear exists of probabilistic approaches that require different styles of interpretation from traditional techniques. More data is required to support model needs.

Holland discussed why modeling and simulation are not widely used, even with established techniques. Reasons include lack of, or inadequate, training resources; time restrictions imposed by aggressive clean-up schedules or contracts; a perception by regulators that modeling is not needed; inadequate site data to construct models; and poor model credibility due to past misapplications. He proposed the following steps toward a more positive direction:

- Decision makers need to know how to use modeling and simulation as a component of decision making.
- Modeling must be viewed as an integral part of the answer, an integral part of an environmental endeavor from beginning to end.
- We need to be clear that modeling involves data gathering.
- We need to move toward a single computational environment.
- We should make more use of GIS-based visualization tools.

Academia. Professor Lester Lave, from Carnegie Mellon University, emphasized the need for full, “cradle-to-grave” life-cycle analysis tools that are cheap, real time, and reliable. He discussed the fate of environmental discharges, information requirements of decision makers, and the need to internalize externalities. Lave discussed at length the issues surrounding the credibility of models and tools. Science tends to focus on uncertainties, the ability to replicate results, and errors of omission. The public, on the other hand, makes decisions about the acceptability of models based on values, critics, and communication (or the lack thereof).

DOE/EM. Caroline Purdy, Program Manager, DOE/EM/Office of Science and Technology, briefly reviewed the history of modeling in the programs with which she is associated. She pointed out that it is important not to “oversell” modeling for a given problem. Future important directions include process modeling (coupled multiphase, multicomponent, non-isothermal, stochastic, and fracture flow processes) and numerical techniques (parallel processing, discretization techniques).

EPA. Subhas Sikdar, director of the Sustainable Technology Division at the EPA National Risk Management Research Laboratory, said that within EPA, modeling and simulation is used to formulate and enforce regulations related to remediation, control/mitigation, pollution prevention, assessment, and cost modeling. EPA priority areas include:

- Human health and ecological risk assessment
- Health and ecological impact characterization—acid rain, ozone, greenhouse gas
- Life-cycle analysis—order of magnitude judgment
- Cost models for Superfund, drinking water, control technologies, and biomass utilization
- Process simulation and integration with environmental concerns
- Material substitution—decision support tools (an expanding field)

Sikdar said that possible areas of future emphasis for EPA are:

- Process synthesis, computational chemistry
- Social-economic models for regulatory strategies
- Industrial ecology
- Ecosystem restoration
- Adaptation (e.g., to global warming)

Question and Answer Period

Following the panel discussions, the panelists answered questions from the audience, as paraphrased below.

1. Why do managers fail to emphasize communication, sell importance, and stress benefits? Is there a misperception of lack of need, or of deficiency? What would be some examples of need?

Response: Managers know that problems exist but do not always know how to solve them. Sometimes political appointees need intermediaries to do this; research managers and brokers do this. Modelers must recognize that they serve a need, not abstract truth. We try to sell modeling first, but we should sell the problem solution, with modeling as a part of the solution. We also need to use language that managers understand. We need to communicate the value of using models and we need communicators who do not promise too much and lose credibility.

2. If people want models that are cheap, real time, and reliable, what about validity? How much does validity count?

Response: We should start with a purpose. Prediction drives high-validity requirements, and less so for comparison or for explanatory models. We need to take into account the history, in a single time series, of what could have happened. Validity is necessary for control. Validation without purpose has no limits. In life-cycle analysis, modeling is part of an adaptive management strategy. We build a capability to insert refinements. So far the area of cleanup has not moved toward adaptive models and updating. In life-cycle evaluation there are numerous components. When we make simpler models for life-cycle decisions, we need to consider error versus efficiency. No matter how qualitative the model, for comparison of options for environmental gain, we need to determine whether they are accurate and precise with respect to one another. At every level, the decision is beneficial. In particular cases, when we evaluate a set of models, we should ask whether the model can do what it claims to do. Models are neither valid nor invalid; they are useful or not useful for a particular decision. We must not exaggerate or make unsubstantiated claims.

3. Non-profit organizations place a high value on validity. Is there a potential for such organizations to have models available through public interface? Can these organizations be provided accurate information about how those models are being used and about assumptions?

Response: It is important to make models available. For example, the Navy posts constantly updated results of the San Diego Bay model on the World Wide Web for discussion. There is the issue of proprietary information; not everything can be provided to the public. All models and underlying data should be in the public domain, but this is not always true for life-cycle analysis. Some issues revolve around private data. Another example of proprietary data is the health data of individuals. The issue here is confidentiality as well as contractual issues. We must be careful about how people use models. Their misuse can set back a policy issue resolution by years. We must also be careful about how data is released.

4. What about validity? We try to build models that are realistic. We document assumptions and embed portions of the system into the model. For example, in a liver transplant allocation model, we used various approaches available as part of model.

Response: Fortunately, much validation data is now publicly available from Federal facilities.

Appendix C. Actinides

Actinides Interest Area Team

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Peake, Tom
Romanovski, Vadim
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The discussion within the Actinides interest area group expanded somewhat to include heavy metals. The reason for this slight change is that some of the actinides, such as depleted or natural uranium and thorium, actually behave more like a heavy metal, such as mercury or lead. Although the emphasis of the discussions was on radioactive actinides, many of the issues and concerns and the conceptual construct of source, waste minimization, waste management, environmental remediation, and background or surroundings can easily translate to heavy metal contaminants. This construct is graphically represented in Figure C-1.

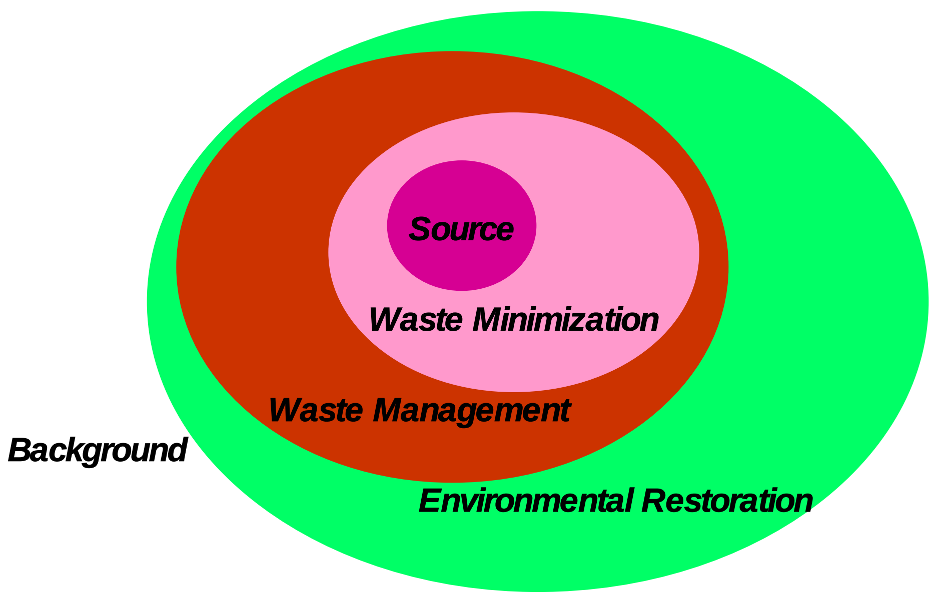

Figure C-1. Activities in which actinides must be managed.

As shown in Figure C-1, there are several specific areas in which modeling should play an integral role. The source term may be associated with chemical processing, actinide generation in reactor fuel, residues stored at DOE sites, or an uptake by an individual. Except for the last example, all of the other sources then result in some type of waste or subsequent residue being formed. The goal is to minimize the amounts, both of the actinide and the bulk matrix, and characterize the form of the waste. As long as waste is being generated, some type of inventory management is needed for waste management. This is also the case for existing DOE sites that already have stored wastes. Environmental remediation cannot be achieved until the inner rings shown in Figure C-1 have been adequately controlled to allow decontamination and decommissioning (D&D) of equipment, facilities, and sites. Ultimately there is a need to model the background (the area outside the rings in Figure C-1) in order to understand large-scale issues such as contamination of immense areas due to fallout (Chernobyl is an example) or due to possible widespread dispersion of materials during D&D activities.

Each of the areas represented by the rings in Figure C-1 have several issues associated with the existing and potential applications of modeling and simulation. Areas that were identified include health effects; data availability and associated uncertainty; conceptual models to assist in problem definition and scope; and identification of needs by decision makers so that models and simulations can help address those needs. As part of working through these issues for each of the areas, the team developed a matrix format (Tables C-1 and C-2). The column headings in these tables are the four areas of concern identified in the previous paragraph; the row headings are the five application areas identified in Figure C-1. This tabular format was used to identify applications (Table C-1), users of the models and resulting information (Table C-2), and existing models being used in these areas.

Table C-1. Applications of modeling to target areas

Application Areas	Health Effects	Data Availability/ Uncertainty	Conceptual/Scope/ Problem Definition	Communication/ Identification of Needs/ Requirements
Source	workers safety public impacts criticality	chemical (thermodynamic, molecular) materials characterization	criticality materials process (small to integrated) near term	process (integrated) sensitivity cost/benefit life cycle analysis
Waste Minimization	workers public	chemical materials characterization	near term waste mgmt	sensitivity decision cost/benefit life cycle analysis
Waste Management	workers public	chemical materials characterization temporal	near term long term gw flow models atmospheric surface hydro reactive transport	interim mgmt disposal cost/benefit life cycle analysis
Environmental Restoration	workers public ecology atmosphere ground water surface water	chemical materials characterization temporal	near term long term gw flow models atmospheric surface hydro reactive transport	waste mgmt disposal no further action cost/benefit
Background/ Contamination	public ecology atmosphere ground water surface water	chemical materials characterization temporal	long term gw flow models atmospheric surface hydro reactive transport	cost/benefit

Table C-2. Users of models and modeling results.

Application Areas	Health Effects	Data Availability/ Uncertainty	Conceptual/Scope/ Problem Definition	Communication/ Identification of Needs/ Requirements
Source	workers public mgmt (operations) DOE-DP	experimentalists modelers operations mgmt (technical)	modelers mgmt (technical & contractor) DOE	public regulators (NRC, DFNSB) mgmt (contractor) DOE
Waste Minimization	workers public mgmt (operations) DOE	experimentalists modelers operations mgmt (technical)	modelers mgmt (technical & contractor) DOE	public regulators (State, EPA, NRC) mgmt (contractor) DOE
Waste Management	workers public mgmt (operations) DOE	modelers operations mgmt (technical)	public modelers mgmt (technical & contractor) DOE	public regulators (State, EPA, NRC) mgmt (contractor) DOE
Environmental Restoration	workers public mgmt (operations, technical) DOE	experimentalists modelers operations mgmt (technical)	public modelers mgmt (technical & contractor) DOE	public regulators (State, EPA, NRC) mgmt (contractor) DOE
Background/ Contamination	workers public mgmt (operations) DOE	experimentalists modelers operations mgmt (technical)	public modelers mgmt (technical & contractor) DOE	public regulators (State, EPA) mgmt (contractor) DOE

Perhaps the greatest area of concern, aside from the health issues that were dealt with in detail by the Health and Ecological Effects interest area teams, was the lack of general actinide and site-specific data for modeling everything from fundamental chemistry to large scale repositories such as the Waste Isolation Pilot Plant (WIPP) or Yucca Mountain. This lack of data, both in the areas of thermodynamics and chemical behavior and potential interactions with site-specific soils and minerals, was viewed as a major shortcoming of the current modeling activities. Several constructive suggestions were put forward to help alleviate this dearth of information.

It appears that there is actually a significant amount of information within DOE, DoD, EPA, and other government and private organizations. However, there is minimal funding currently being applied to gathering, collating, and entering this information into a data base in a form that is accessible and usable by the modeling community. This issue is addressed in one of the recommendations from the Actinide interest area team.

A wide variety of modeling packages is currently being used to simulate actinide behavior. This has led to concerns about the appropriate use of these models and the reliability of the information resulting from their use. Because of the uniqueness of the actinide problem, many models have been developed that were intended to address either specific questions, or to be used for relatively specific and narrow applications. Many of these models have been used on a much expanded basis. Further, there are some areas for which models may not currently exist, either because of the extreme complexity of the problem, a lack of information upon which to construct a conceptual model, or a lack of clearly defined needs so that specific information can be inferred from the model results.

Finally, the overarching problem of a consistent approach to developing and using a set of needs (information required to assist in making an informed decision) to lead to a well defined scope and problem has resulted in inconsistent use of models and skepticism about model results. Before existing models can or should be used to address specific issues, there is a need for a conceptual model that helps give definition to how the overall information generated by modeling and simulation will address the problem definition and, in turn, provide useful, understandable information for the requester who must make some type of decision.

Appendix D. Decontamination and Decommissioning

Decontamination and Decommissioning Interest Area Team

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Petullo, Colleen F.
Roberts, Randy

The Decontamination and Decommissioning (D&D) interest area team discussed the importance of modeling and simulation in the D&D area, why it was important, and what needs to be done in business processes, in identifying and realizing $8M in efficiency improvements in the 2006 Plan, and optimizing cost, schedule, and engineering. An assessment needs to be made of available business processes in DOE, other federal agencies, and private industry (Fortune 500), and we need to adapt or adopt dose and risk-based criteria for the release of facilities and equipment. In assessing available models, we need to determine how they are being applied (interfaces), how the job can be done better, and whether integration can be improved. In optimizing factors such as cost, schedule, and engineering, we need to capture and evaluate lessons learned, integrate existing efforts and capabilities, and evaluate existing modeling efforts.

Questions and Answers

The team discussed and answered the twelve questions presented as guidance for the workshop participants.

1. What are the important problems to be addressed by modeling and simulation? Political? Societal? Economic? Environmental?

Discussion: D&D cross cuts many of the workshop interest areas, including:

- Subsurface Contaminants
- Health and Ecological Effects
- Infrastructure
- Waste Treatment
- Actinides
- Manufacturing/Pollution Prevention

D&D modeling and simulation must consider economics (life cycle cost; mortgage reduction), safety, environmental regulations, societal (stakeholders), political (stakeholders), risk/uncertainty, regulatory/compliance, holistic view point (integration), and technical (engineering approach; technology selection).

2. Which questions in this area can be answered with models?

Discussion: Intelligent integration of all the elements must be addressed because D&D cross cuts so many areas and considerations. The decisions that modeling and simulation can address depend on the decision types/levels (tiered decision process). After considerable discussion, the team developed a framework to describe the various decision types and levels, and indeed the key decision makers. This framework is shown in Figure D-1. In this pyramid, the apex (Level A) consists of senior managers located at both headquarters and the field; in the middle (Level B) are mid-level managers at both headquarters and the field; and at the base (Level C) are D&D project managers in the field.

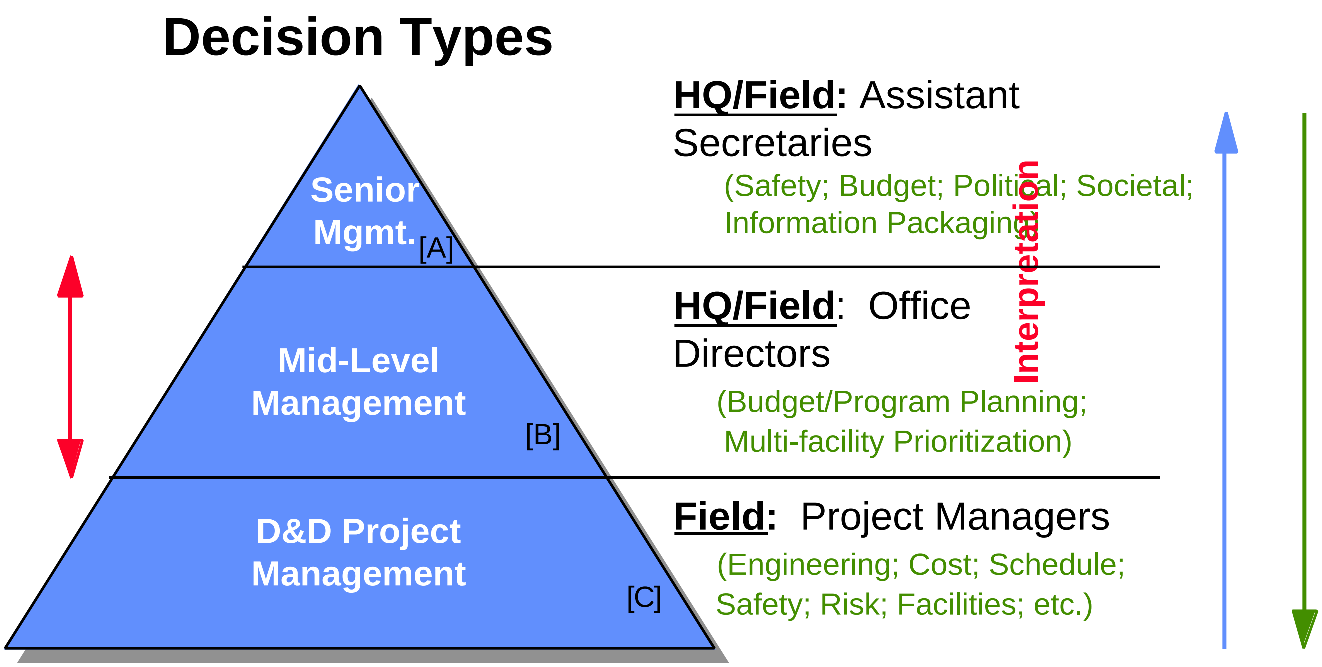

Figure D-1. D&D Modeling and Simulation.

· Level A—Senior managers at Level A include assistant secretaries and deputy assistant secretaries at DOE headquarters. In the field, they include DOE Operations Office managers and assistant managers, especially the Assistant Manager for Environmental Management. Also included are the presidents of site contractor organizations. They are focused on safety, budget, political, and societal issues and concerns. They need to organize and manage a tremendous amount of information in order to make informed, defensible decisions. Information packaging is critical to these decision processes. Business processes and practices are key to their success.

· Level B—Mid-level managers at Level B include office directors and D&D program managers at DOE headquarters. In the field, they include DOE Operations Office environmental restoration managers and D&D program managers. Also included are environmental restoration managers and D&D managers in site contractor organizations. They are focused on D&D program and budget planning for an entire DOE site or a geographic grouping of sites. Models that allow prioritizing all site D&D activities in accordance with regulatory, risk, etc. could be useful. This could be labeled multifacility prioritization at a site.

· Level C—D&D project managers in Level C are located in the field, typically in the site contractor organization or in commercial D&D firms for outsourced D&D projects. They are focused on detailed project planning and execution(engineering, cost, schedule, safety, manpower, etc.) for a single facility, perhaps a single building. Models at a more detailed level are useful. The questions at this level are more technical and detailed in nature.

3. What is the size/imminence of this problem?

Discussion: The team considered this question within the context of the pyramid model. The magnitude of the problem at Level A is very high. Annual and multi-year decisions are the norm. Within DOE-EM, the 2006 planning process is underway with annual budgets of approximately $6 billion; D&D encompasses approximately 7,000 facilities with projected costs of approximately $20 billion, 90% of which will occur after 2006. There are plans to completely remediate three DOE sites (Rocky Flats, Fernald, and Mound) by 2006. Within the Nuclear Regulatory Commission (NRC), 12 of the 109 commercial nuclear power plants in the U.S. are shut down and awaiting decommissioning at a cost of $350 million to $400 million each. With the advent of electricity deregulation, early decommissioning of many more nuclear power plants is expected prior to the end of their operating license period.

At Level C, D&D is ongoing and immediate. Life-cycle cost savings are needed now. Outyear D&D mortgage reductions are needed now. At this level, detailed databases and models are particularly useful. Relative to the decision makers' pyramid, D&D activities include:

- Level A (senior managers): 2006 plans, detailed annual budgets, and external and internal urgent actions (fire drills).
- Level B (mid-level managers): Program planning/budgets site wide, operable units, and information requests from Level A.
- Level C (D&D project managers): Facilities (individual buildings); detailed project plans that encompass cost, schedule, engineering etc.; site specific issues/concerns; and information requests from Levels A and B.

The regulators (federal and state) and stakeholders are integral to the process at all three levels. Any model needs to be able to incorporate all these entities and elements. Information is rolled up from Level C (details on individual facilities) to Level B (details on a site or geographic grouping of sites) to Level A (the DOE Weapons Complex). This process is represented in Figure D-1 by the arrow pointing up from C to A. The arrow pointing down from A to C represents the policy and guidance flowing down, including decisions representing political and societal perspectives.

4. What is the current level of effort toward solving the problems?

5. Have modeling, simulation, and analysis been used to address problems in this interest area, and if so, which ones and how effectively?

Discussion: The participants found it useful to consider these two questions together, rather than sequentially. Most of the current effort is occurring at Level C. Senior and mid-level managers require rolled up information to enable informed, defensible decisions. While considerable detailed information exists in a variety of databases and information libraries, integrated models and simulations are virtually nonexistent; there is little capability to optimize this information in a useful manner. At Level C, models exist for individual parts of a D&D project:

a. Engineering cost estimates

- MCACES (U.S. Army Corps of Engineers)
- INVEST (US DOD)
- RACER (commercially available)
- Various propriety commercial models (Project Performance Corp., Project Time and Cost, TLG Associates, NES, Inc., and others).

b. Risk assessments (models available now)

- RESRAD
- RESRAD-Build
- RESRAD-Recycle

c. Optimization of cost, schedule, engineering, etc. The Phoenix Model (under development)—The D&D Focus Area (DOE-EM OST) has funded an effort intended to provide a framework and capability to optimize a D&D project based on all the necessary elements (e.g., cost, schedule, risk). This effort is still in the early development stage.

d. Waste minimization/pollution prevention

- RESRAD-recycle for metal
- Vanderbilt University's systems study on concrete recycle (in progress now; funded by the D&D Focus Area).

D&D project manager responsibilities

The D&D project manager is responsible for surveillance and maintenance, including the development of the D&D plan, which deals with the project, safety, planning, technical approach, environment, possible outsourcing of the actual work, and performance of the work that occurs within the site organization. Worker protection and proper selection of personal protective equipment are integral to the project. Characterization, decontamination, dismantlement, material disposition/recycling, final characterization activities, and extensive documentation throughout the project are key responsibilities of the project manager. The D&D project manager has many information resources to draw on:

(1) DOE-EM Office of Environmental Restoration (EM-40)

- Decommissioning Handbook
- Preferred Alternative Technology Matrix
- Benchmarking Study
- RAPIC Library (prior D&D project documents)
- National Decommissioning Committee

(2) DOE-EM Office of Facility Transition and Material Stabilization (EM-60)

- Deactivation Handbook
- FASTER (under development to capture and disseminate lessons learned for successfully completed deactivation projects)

(3) DOE-EM Office of Science and Technology (EM-50)

- D&D Focus Area (technology development/demonstration)
    - Web Page
    - Large-Scale Demonstration Projects (technology demonstration fact sheets, innovative technology summary reports, technology implementation/deployment fact sheets, web pages)

(4) NRC Decommissioning Information (Nuclear Power Plants and SDMP's)

- Web Page
- Rulemaking and guidance
- D&D (framework for final release from license)
- D&D Plans (for individual nuclear power plants)

(5) Information Management

- STREAM (commercially available from Delphinus Eng.)
- 3D visualization of facilities (includes virtual reality)
- Contaminant mapping (3D-ICAS under development in EM-50)

(6) Integration

- Decision Analysis (includes expert systems)

(7) Facility release criteria

- RESRAD (land)
- RESRAD-Build (buildings)
- D&D (release from NRC license)
- MARSSIM (a final site survey characterization decision tool)

(8) Release of Equipment/Material

- Resrad-Recycle (Metal)
- EPA uses a spreadsheet approach
- NRC uses a methodological approach
- IAEA has issued for comment a report with release criteria
- Vanderbilt University's systems study on concrete recycle

6. What can be done with modeling, simulation, and analysis in this area?

Discussion: RESRAD has been widely applied and accepted. RESRAD-Build is being applied at:

- EBR-II at ANL
- HWCTR at Savannah River site
- 105-C production reactor at Hanford
- Grand Junction facility

RESRAD-Recycle is being applied at:

- Release of nickel at Paducah site (potential sale to Spain)
- Release of copper ingots at Fernald site
- CP-5 research reactor case study at ANL

STREAM is an information management tool that allows a D&D project manager to efficiently plan and execute a D&D project. With its multimedia capability and use of a variety of spreadsheets, STREAM captures, organizes, and portrays information on the facility, contaminants, engineering approach, and other factors such as schedule, costs, manpower, and waste management.
STREAM is being applied at:

- 105-C production reactor at Hanford
- HECTR facility at Savannah River Site
- Chernobyl project in the Ukraine

All codes applied to subsurface contaminants (ground water and soils) are important and integral to a D&D project. The team defers to the discussions of the Subsurface Contaminants interest area teams for details. Air Pathway Exposure Codes and other fate and transport models for other pathways (e.g., risks to health and the environment) are integral to D&D projects. The team defers to the discussions of the Health and Ecological Effects interest area teams for details.

In the area of engineering cost estimation, proprietary capabilities in the commercial sector are being applied at:

- Project Performance Corp.
- Project Time and Cost
- NES, Inc.
- TLG Associates
- Individual D&D contractor firms

Government capabilities are being applied at:

- Federal Remediation Roundtable
- MCACES (US Army Corp of Engineers
- HCAS (Historical Cost Analysis System)
- DOD INVEST (now commercially available as RACER)

The Yucca Mountain Options Study is an example of a systems study that was a technical success, but a political/societal failure.

7. If modeling and simulation is not being used, or not being used successfully, why not?

Discussion: Decisions are being made at all levels whether models are available or not to aid the decision making process. In general, there is a lack of standardization of approaches, but efforts are underway to rectify this. Each site uses its own system and it is difficult to easily transfer data or models. In the cost arena, there is a lack of a standardized approach across DOE sites. Project EM (currently underway) is an attempt to standardize the cost methodology used across the DOE Weapons Complex. Project EM is led by the DOE-Federal Energy Technology Center's EM Center of Excellence for Acquisition and Business Excellence (CABE) with substantial participation by the U.S. Army Corps of Engineers and other entities.

Some of the reasons hindering the usage of models and simulations include the fact that the model user is not connected to model development; there are disagreements on how to deal with uncertainty; and the lessons-learned process is inefficient.

8. Is there a gap between the development or models and simulation tools and methodologies and their application?

Discussion: Two aspects of application are (1) usage, which includes training, defining the appropriate problem, interpretation of results, and user-friendly interface, and (2) interfaces with other elements of the decision process with appropriate linkages.

The RESRAD codes have been modified as gaps have been discovered. Validation and verification of new codes is extremely important. The Phoenix model, which is in the early development stage, is not well connected to the EM-40 D&D program, especially at the headquarters level. A rigorous review of this effort should be performed before any further development work is undertaken.

Referring to the previously discussed decision type pyramid in Figure D-1, a gap exists in how to reconfigure, repackage, and present information moving up or down the pyramid to and from Level C through Level B to Level A.

9. Have there been cost/benefit studies for various models and simulation, and analysis tools and methodologies?

Discussion: An effort has been made to determine the benefits of using specific RESRAD codes. The participants on this interest area team were not aware of cost/benefit comparisons of competing models. Individual models have been used to compare options for a particular D&D operation.

A good payoff is expected if Mod/Sim efforts are expanded and integrated/standardized if the focus is on the following areas:

- Life-cycle system engineering should pay off in reduced cost, shortened schedule, and reduced risk for a given facility.
- Reducing uncertainty in data and in decision making should translate to payoffs in cost, schedule, and risk.
- Mortgage reduction in the outyears should be substantial.

10. What modeling and simulation techniques are shared with other interest groups?

Discussion: Visualization/management (packaging) of information applies to senior managers at Level A and mid-level managers at Level B. This really cuts across all organizations in DOE (EM, DP, EH), DOD, EPA, NRC, and applications such as waste minimization, pollution prevention, and environmental media models. Techniques are needed for direct staff to an assistant secretary to manipulate databases to best package/portray rolled up information.

Business processes and practices are needed. NRC calls its effort in this area Business Process/Reengineering (BPR). A recent article in the C&E News issue of 9/15/97 discussed the systems used by many major chemical companies. The generic term for these information systems is Enterprise Resource Planning (ERP). In the chemical industry, ERP tools are used to maintain the gains of business process reengineering, realize the promise of supply-chain optimization, and create a truly global enterprise. By creating a centralized database and standardizing corporate data flow, ERP can make changes and efficiencies take hold in a company. Proprietary ERP tools are commercially available (offered by SAP, Oracle, J.D. Edwards, SSA, Intentia, and others), and should be assessed to determine if their adoption or simple adaptation can meet the needs of a government organization such as DOE-EM. The current DOE-EM 2006 plans require identifying and realizing $8 billion inefficiencies on a base of $60 billion; ERP has the potential to make a substantial contribution to meeting this challenge.

11. What are the other benefits that can be obtained from modeling and simulation?

Discussion: Modeling and simulation helps to control cost, schedule, risk, and uncertainty. It helps in developing performance-based contracting, setting performance specifications, and privatization.

12. What measures can be used for assessing how well modeling, simulation, and analysis are being applied?

Discussion: Performance measures must be established both for existing models and for potential development of new models. In establishing performance measures, the following questions must be asked: What are the returns on investment? Is this an enabling technique not otherwise available?

In the transition from absolute standards for cleanup to dose-based guidelines derived from modeling, there is a need to incorporate site-specific data to reduce conservative generic approximations; optimize baselines to optimize cost/schedule; and minimize data collection.

Again, it is important to understand that the DOE-EM 2006 Plans require $8 billion of efficiencies to be achieved during the ten-year period on a base of $60 billion. Can modeling and simulation efforts contribute to identifying/realizing the $8 billion in efficiency improvements? Both the "Necessary and Sufficient" process and the "Work Smart" process can contribute to these required efficiencies.

Three essential questions for all modeling and simulation efforts are:

(1) Do (will) the regulators accept it?

(2) Do (will) the stakeholders accept it?

(3) How user friendly is it?

In general, modeling and simulation can:

- Reduce decision error or quantify decision risk
- Optimize cost/schedule/engineering
- Minimize new data collected

Efforts should focus on the interface between Level A (business) and Level C (science and engineering), and on business processes and practices.

The Sandia Environmental Decision Support System (SEDSS) provides an integrated decision-making methodology and an automated computer-based tool based on that methodology. The purpose of the methodology is to direct risk assessment, remediation selection, licensing, site characterization, and monitoring based on the potential risk to human health and the environment and on the cost of alternatives.

The objectives of the SEDSS are to automate the analysis, thus allowing the decision maker to focus on the decision, ensure the consistency of approaches, document the decision process, reduce loss of information between steps, provide an improved basis for negotiation and conflict resolution, and save time and money. The SEDSS is designed to incorporate probabilistic methods for evaluating site safety or remedial options into a decision framework for the purpose of:

- Accommodating the effects of uncertain site-specific information
- Balancing the costs versus benefits of site data collection
- Facilitating a consistent decision approach across all involved or affected parties.

The SEDSS project has set the following strategies: (1) to create a defensible and robust decision support framework (referred to here as the Decision Framework) and define in detail how to address each step of the process in a way that allows for continued improvement; and (2) to automate the Decision Framework into a user-friendly software tool. The process of following the Decision Framework using the software tool results in a consistent application of the methodology and a documented trail of assumptions that can be the basis for negotiations. The use of the tool will allow for the decision making process to be faster, more consistent, better documented, and less costly.

The SEDSS methodology is designed to assist in risk and resource management decision making and can be applied to a variety of environmental and exposure pathways involving both radionuclide and hazardous contaminants. With the capabilities provided, decision makers can more effectively address the following types of environmental decisions: Is the site safe? What remedial approach should be used? When is the remediation complete?

The underlying methodology is designed to use an iterative analysis approach that incorporates forms of probabilistic environmental fate and risk analysis, cost/benefit analysis, and site-sampling optimization techniques. This provides a quantitative estimate of risk to human health and/or the environment with an explicit treatment of the uncertainty associated with these estimates. Results of the risk analysis can be used to direct additional site characterization and monitoring activities, as well as provide a consistent framework for comparing alternative system conceptualizations. Within this iterative approach, new data are collected only if necessary and cost effective. These data are then used to update our understanding of the system and reduce uncertainty in decisions.

To support the decision analysis, the SEDSS is designed to capture and store user input data and link to site information, guide the user through the process of developing a site conceptual model based on available information, evaluate the conceptual model with physical process models, allow explicit comparison of results with a performance objective, and identify additional data needs and/or design remediation schemes.

To date, the software has automated the Decision Framework for setting Performance Objectives, establishing existing information (e.g., information in a GIS), defining the Conceptual Model, running a limited set of code capabilities in a Monte Carlo process, and displaying the Performance Decision Point that will allow the user to determine whether a decision can be made or if it is necessary to continue through the rest of the Decision Framework steps, conduct Sensitivity Analysis, and conduct Data Worth analysis.

Current funding organizations include the EPA, the Office of Emergency and Remedial Response (Superfund), the Office of Radiation and Indoor Air, the Nuclear Regulatory Commission, Office of Research, Waste Management Branch, DOE, and the Uranium Mill Tailings Remedial Action Program.

SEDSS has been developed under object oriented software architecture that will allow for future expansion. The entire development process is being conducted using industry standard software quality assurance and configuration management methodologies. The software is written in C++ and the numerical and analytic codes are currently in FORTRAN. The graphical user interface (GUI) is built using MOTIF and MOTIF standards. SEDSS is currently available on a SUN or SUN Server. A PC version is planned for FY97.

Appendix E. Environmental Security

Environmental Security Interest Area Team

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The Environmental Security interest area team agreed that models being discussed by other interest areas at the ModSim'97 USA workshop could be readily applied to environmental security issues. The model development required for the environmental security interest area includes:

1. Coupling the phenomenological models with each other.

2. Linking the coupled phenomenological system with the social systems models.

3. Creating higher-level models that include key processes and feedback for decision makers.

The participants were not sufficiently familiar with the social systems models to comment on the amount of development required for these systems. The models for environmental security should include feedback because the feedback may significantly affect the results and, consequently, the acceptability of the proposed solutions.

Communication was identified throughout the workshop as being a key issue for model development and application. The end user, in particular the policy maker, needs to be included at early stages of model development, and the involvement should be continuous so that the model is relevant and its limitations are understood. The results must be obtained in a timely fashion so that the time for the required decision has not passed when the results are ready.

Technical developments are coming online that will facilitate the development and application of the coupled models required for environmental security. Computer speeds of a teraflop will be realized in the next few years. In addition, computer memory and the programming environment will be enhanced. Large databases will be needed for model testing, and the computing environment will allow more rapid access and integration of these databases. Presentation of the results in terms of visualization was identified as critical for higher-level decision-makers. High-speed communications for model and data transfers are being developed and these transfers are crucial to both sides having the same information to resolve the issue. Finally, the advent of the Internet was identified as a technology that not only facilitated the transfer of information, but also allowed the establishment of fundamentally different working relationships—people no longer have to be collocated to participate in effective working groups.

Internationally accepted environmental security models will produce significant benefits by:

- reducing political uncertainty and increase stability
- identifying areas for intervention before they become critical
- guiding allocation of resources for data collection
- pointing to areas for development in the models needed to better address policy issues.

Questions and Answers

The team reviewed the twelve questions given to the interest area teams for discussion, and answered the questions as follows.

1. What are the important problems to be addressed by modeling and simulation? Political? Societal? Economic? Environmental?

Discussion: The group reached a consensus that transboundary transport of contaminants was a primary environment problem for environmental security. Other environmental security issues included facility design and operation, problems of natural resource use, common areas such as the oceans, Arctic and Antarctic, natural disasters, global climate change, and mitigation of future problems.

2. Which questions in this area can be answered with models?

Discussion: All of these issues can be addressed, but in many areas the basic understanding, the data, and/or the modeling framework are missing.

3. What is the size/imminence of this problem?

Discussion: The discussion of this question was lively and the answer is that “it depends” on factors which may be outside of the environmental area. This conclusion is a recognition of the fact that in many cases environmental issues will increase the background stresses on the populations, but crisis or conflict will be triggered by some other event.

4. What is the current level of effort toward solving the problem(s)? When is enough?

Discussion: In some instances such as Europe, lead institutions have been established for projects such as Norway for No_x and So_x and Russia for organic compounds. In the U.S., DOE, DoD, and EPA have signed a Memorandum of Understanding (MOU) in this area, but the efforts tend to be focused on existing problems. Modeling efforts are spread across a number of disciplines. What is needed is the integration (in the context of environmental security) of information and experimental data.

5. Have modeling, simulation, and analysis been used to address problems in this interest area, and if so, which ones and how effectively?

Discussion: The team discussed a number of model types, as shown in Figure E-1.

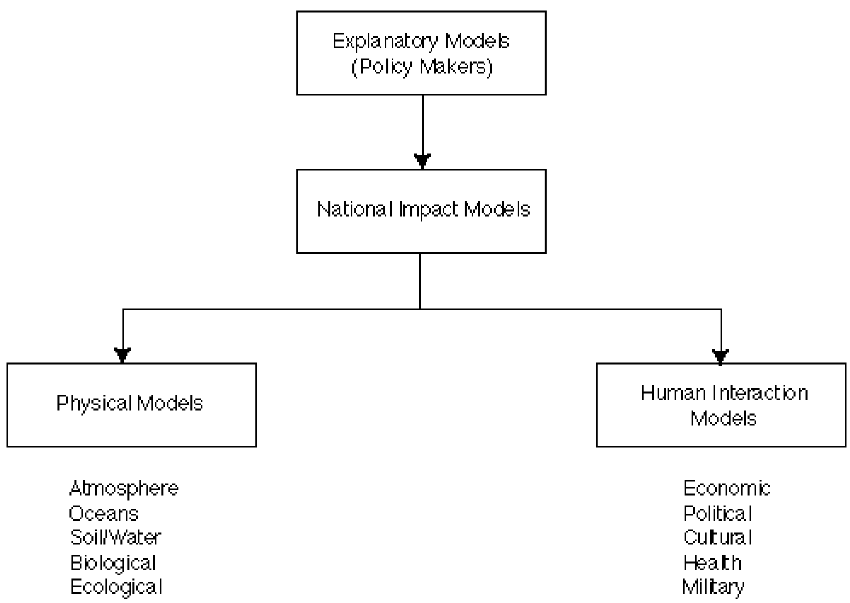

Figure E-1. Environmental Security Model Types

Atmospheric models have been used for accident scenarios, volcanic eruptions, explosive emissions, and atmospheric pollutant transport. Biological models have been applied to tracking disease and the health impacts of radiological releases. Ocean models have been used for fisheries. An extensive number of models exist for chemical transport through soils. The physical and human interaction models must be coupled and linked to account for critical feedback between systems.

6. What can be done with modeling, simulation and analysis in this area? (Examples, success or non-success stories)

Discussion: Successful model applications include the prediction of environmental consequences from the Persian Gulf War and studies of accident scenarios. Unsuccessful attempts are the acid rain program that delivered the answer too late and an example from Rio de Janeiro. The importance of communication and proper initial conditions in modeling was underscored by the modeling of the recent flooding in central Europe. The lack of data sharing between countries caused a downstream model *not* to predict the floods. If the data and operation rules for the reservoir had been known, the floods would have been predicted.

7. If modeling and simulation is not being used, or not being used successfully, why not?

Discussion: Factors that prevent model use in the environmental security area include the limited capabilities of the models in this area; the decision makers' lack of familiarity with the existence, limitations, and value of the existing models; the modelers' lack of awareness of the needs of the decision makers; computing limitations; the lack of an identified sponsor; the diversity of efforts included under the title of environmental security; and lack of ownership by the end user (policy maker).

8. Is there a gap between the development of models and simulation tools and methodologies and their application? Are new models, tools, and/or methodologies needed?

Discussion: Interfacing physical models with human interaction (social) models will be a major challenge. Enhanced computational capabilities need to be more widely and readily available. Customers want rapid answers, so off-the-shelf tools are used instead of developing new, more sophisticated tools. Multinational efforts are needed to evaluate data and models and increase access to the environmental data collection capabilities of the intelligence communities. Forecasting of natural disasters is another area that needs further development. The Chinese have an informal union of scientists involved with environmental assessment, and there was a suggestion for a multinational effort in this area. The International Academy of Ecology and Security (IAEA) has the BIOMASS group on modeling.

9. Have there been cost/benefit studies for various models and simulation, and analysis tools and methodologies? Do we expect a good payoff if efforts are expanded into modeling and simulation?

Discussion: There is no direct application of cost/benefit to environmental security models. Modeling and simulation have been used to direct efficient data collection; may be used to design regulations; and, as a component of environmental treaty verification, may be used as a tool in developing real-time control systems.

10. What modeling and simulation techniques are shared with other interest groups?

Discussion: Models developed by the other interest areas can be applied to environmental security, as well as tools developed for the social sciences, which were not represented at the workshop. Special emphasis should be placed on the coupling of models. When models are coupled, special attention is needed on how the uncertainties are propagated from each model through the coupled model structure. Model accuracy is critical and uncertainties within the models being coupled need to be tracked through the coupled system.

11. What are the other benefits that can be obtained from modeling and simulation?

Discussion: Numerical and mathematical models have the potential to largely replace experimental and field monitoring activities. Many of the computational resources (hardware and software) are already available to solve many of these problems. Good models reduce uncertainty and increase international stability. Models can support the deployment of monitoring systems, making them more cost effective. They can guide the interpretation of data that are acquired and provide a basis for better scientific understanding. Construction of the models and analysis of their output may identify situations or conditions that were not originally recognized as being present in the real system. Joint model use and understanding increase confidence and stability between countries. Models can also be used to simulate future events.

12. What measures can be used for assessing how well modeling, simulation, and analysis are being applied?

Discussion: The comparison of predictions to data is the basic metric that evaluates a model from a scientific perspective. The data can consist of observations or the results of theoretical studies or other modeling efforts. Models can be used in a relative fashion to compare scenarios and measure change rather than to create accurate predictions. Sharing of data across boundaries will make model applications more efficient and practical as a tool to resolve issues related to environmental security.

Recommendations

The recommendations made by the Environmental Security interest area team are as follows:

- Combine the models of physical (natural) systems and human interactions (policy and social issues) for this interest area.
- Develop and use coupled models for global, regional, and local scales.
- Focus on interfaces within and between models (integrated models).
- Develop the ability to handle different scenarios that include a variety of different time scales and measurement parameters.
- Develop a common international reference for models and data, including metrics (which can be driven by cooperation within the scientific community).
- Exploit increased computational capability; develop mathematical algorithms, GIS systems, and improved analytical techniques to better analyze data, model, and improve access to data.

- Incorporate the models proposed by other interest groups wherever possible.
- Stress effective communication at all levels (modelers to policy makers) and at all stages (design to end use). Results must be relevant to, and understood by, policy makers.
- Involve end users early in the process.
- Develop cost/benefit systems for environmental security problems.
- Improve data and increase access to data sources.
- Validate and seek acceptance for models in order to reduce uncertainty, increase stability, point to new scientific directions, and guide new data collection.

Appendix F. Health and Ecological Effects I

Health and Ecological Effects I Interest Area Team

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The mission of the Health and Ecological Effects I interest area team was to answer the question, "What is the role of modeling and simulation in estimating effects to humans and ecological receptors?" The team considered the role relevant to the following:

- Estimating the amount of hazardous material reaching human and ecological receptors.
- Estimating the duration of exposure.
- Estimating the magnitude of adverse effects to humans and ecological receptors.
- Providing risk communication tools.
- Providing the means to support decisions and foster environmental stewardship.
- Quantifying uncertainty in estimates and evaluating the sensitivity of models and model parameters.

Questions and Answers

The team used the 12 questions that were presented as pre-workshop guidance as the focus of their discussion. The results are presented below, including the preliminary discussion that preceded considerations of the questions themselves. While there are similarities between human health and ecological risk assessment (e.g., in terms of pathway analysis), there are differences in terms of endpoints (e.g., toxicology). Also, human health risk is "old," whereas ecological risk is "new." Can they be addressed together? Yes, but the differences must be identified. Also, the discussion must not focus only on radiological issues, even though previous risk assessment work has tended to focus in this area until relatively recently.

1. What are the important problems to be addressed by modeling and simulation? Political? Societal? Economic? Environmental?

Discussion: There are problems with the toxicological data base for ecological risk. Appropriate toxicological data often is not available. Many limits are based on studies that are not applicable to natural situations. Ecotoxicological studies would be desirable. There are also conflicting goals of regulatory compliance and assessment of ecological impacts.

How does risk assessment apply to D&D? Many regulatory limits are based on an early reliance on technology limitations. The situation has changed. We now need to use new tools that will predict exposures and the effects of exposures in order to predict risk based on the real world. This may have to be done on a site-specific basis. Modeling can help in giving us these answers. We need dynamic tools applied across systems as opposed to statistical treatment of data and empirical relationships. Many regulations are targeted toward certain contaminants in isolation (stovepipes). We must consider exposure to mixes of small quantities of many chemicals as well as multiple stressors. There is a need for integrated environmental management.

We must look at larger scales and integrated systems. Questions that need answers are: What do we value in a system? What do we want to protect? What are the endpoints? How do we reach consensus? Do models have to be tailored to specific situations, with different models for different purposes? How does life-cycle analysis relate to this? Do all of these models fit within life-cycle analysis? How do you reach consensus on the use of models? Can models be used to demonstrate compliance with regulations?

Uncertainty must be addressed, both in terms of variability of data and in terms of lack of understanding. Models can be used to understand how a system operates. Models also can be used as teaching devices. Consider model-data linkage and the role of models in designing data collection processes. Most environmental data have a half life of 2-3 years. The data collection process/design should take this into account.

There are many assumptions and limitations on available data. There is a need to develop large scale integrators. The money being spent on risk assessment is being spent very inefficiently. Communication of risk is an important aspect of risk assessment. Models can be used to assist in visualization of risk. Human health risk results and ecological risk results can be at odds.

Models can be used to assist in making decisions. Is that the important question? What is use of models in setting priorities? A longer term commitment to models/modeling is needed.

How do we link toxicological data on systems to large field-scale effects on populations? How can models be used to help establish sampling designs (what and how often) on limited budgets? Is sustainability possible? When will we reach the point of no return?

Most money being spent for environmental protection is not protecting our environment. Current policy and priorities are often based on anti-establishment and pro-environment attitudes of the 1950s.

There is no “one” answer. People need to learn that every answer is bound by many factors. This education of the public relates to communication. The decision support system must be used to communicate alternatives and possibilities. However, different people will come to different decisions because they will have different attitudes about what is important. We need to remember that the model is separate from the decision process. However, the model can be biased either by design or by the data that are input. Risk is a probability, not a fixed number. There is a general perception that the public does not want to be involved; however, the public is more likely to accept decisions if it is involved from the start of the process. The problem is getting participants who really represent the general public. More often, participants represent special interest groups.

The team listed problems related to this topic:

- Ecotoxicological data bases for ecological risk are inadequate. Are they appropriate for evaluating risk?
- Methods for addressing multiple stressors and integration of risks need development.
- Scaling is an important issue.
- How do we set priorities/objectives? (1) Use priorities to select models. (2) Use models to set priorities. Both are important.
- Long-term commitment is needed if appropriate/adequate models are to be developed.
- Extrapolation from ecotoxicological data to ecological endpoints is inadequate.
- How can we evaluate sustainability without long-term data sets?
- Uncertainty is not yet well represented and is confused with confidence.
- Data on the uptake and transport of contaminants in natural systems is lacking.
- Decision analysis methodology is inadequate.
- How do we set national priorities?

The team identified areas in which models are necessary. Models are needed for:

- evaluating risk and compliance.
- achieving specific goals.
- addressing uncertainty.
- education.
- assisting in data collection and design of sampling.
- cost/benefit analysis.
- assisting in visualization of risk.
- evaluating alternatives.

2. *Which questions in this area can be answered with models?*

Discussion: the team listed the following areas addressed by models:

- Making projections of future conditions (forecasting)
- Adaptive management

- Prioritization of design alternatives
- Decision analysis (includes cost/benefit analysis)
- Retrospective analysis (e.g., exposure assessment)
- Communication, education, and visualization
- Uncertainty and sensitivity
- Design of data collection studies (includes identifying data gaps)
- Life-cycle analysis
- Establishing standards/compliance levels
- Heuristic value

3. *What is the size/imminence of this problem?*

Discussion: Questions to consider include: Are ecotoxicological data bases appropriate for evaluating risks? Can sustainability be evaluated without long term data sets?

Uncertainty is not yet well represented and is confused with confidence. Data is on the uptake and the transport of contaminants in natural systems is insufficient.

Methods for reaching consensus among the public, scientists, and decision makers are ineffective. Communication of what models can and cannot do is necessary. Methods for communicating uncertainty need to be improved.

Gaining public acceptance and credibility for models is a problem. Decision support models and models for making realistic projections are likely to require site-specific data collection and customization of models.

4. *What is the current level of effort toward solving the problem(s)? When is enough?*

Discussion: The amount of support varies widely from discipline to discipline (e.g., geohydrology versus ecological risk assessment). Realization of the necessity for increased emphasis on model development may be growing, at least in some areas. This team decided that this question could not be adequately addressed because of the limited cross-sectional background of the participants.

5. *Have modeling, simulation, and analysis been used to address problems in this interest area, and if so, which ones and how effectively?*

Discussion: Highlights of the discussion abut where models have been used included the following:

a. *Projections of future conditions (forecasting)*

- RESRAD (rad transport model)
- RESRAD CHEM

- RESRAD BUILD (doses inside of buildings)
- RESRAD RECYCLE (recycled materials)
- RESRAD ECORISK (chemical ecorisk screening)
- CalTOX (multimedia chemical human exposure model for EXCEL)
- CAP88 (air dispersion model)
- MEPAS (multimedia chemical model)
- MILDOS (air dispersion model for rad, multisource)
- ICRP and NCRP screening models
- COMPLY (rad air dispersion screening model)
- RISKIND (multimedia chemical human health model for EXCEL)
- AARAC models
- BIOENERGENICS III (predicts organic concentrations in Great Lakes fish populations)
- SWACOM (aquatic ecosystem model)
- FORET (forest simulator model)
- MMSOILS (chemical multimedia soils model)
- PRECIS (probabilistic human health risk effects)
- ISOSHIELD (buried deposits)
- PABLAM (aquatic systems)
- Hanford Aquatic Model (CRITTER?)
- GENII (rad transport)
- EPA Screening Models (spreadsheet models)

b. *Adaptive management* (iterative [“adaptive”] management decision models)

- A process that uses prospective models
- Sensitivity analysis required

c. *Prioritization and design of alternatives*

- Dependent on attributes required
- LIPS (DOE generic prioritization model)
- MEPAS (can be used as a prioritization model)
- HRS (EPA hazard ranking system)
- To some extent, all predictive models can be used

d. *Decision analysis*

- Cost/benefit analysis
- Population viability analysis
- EPA and DOE model databases
- Many tools, such as Crystal Ball, exist to help in decision analysis

e. *Retrospective analysis* (includes exposure assessment, etc.)

- See list of models for item a; most could be used
- PATHWAY (NTS food chain model)
- RATCHET (Hanford air dispersion model, complex terrain)
- ECOSYS (European model)
- BIOMOVS study models (Chernoble study)

f. *Communication, education, and visualization*

- GIS can be used as a tool
- EcoBeaker (ecorisk)
- RAMIS (ecorisk)
- SIM series of models
- All projective models potentially could be used

g. *Uncertainty and sensitivity*

- RESRAD Probabilistic (Monte Carlo for rad)
- CalTOX/Crystal Ball
- PATHWAY
- RATCHET
- BIOENERGETICS III
- PRECIS
- FORET
- SWACOM (?)

h. *Design of data collection studies* (includes identifying data gaps)

- See items a, e, and g

i. *Life cycle analysis*

- RACER (costing model)
- Process uses systems of models

j. *Establishing standards/compliance levels*

- Usually screening level or empirical models are used
- Standards are usually back-calculated from standards or guidelines (e.g., RESRAD)

k. *Heuristic value* (see item f.)

The team identified the following modeling tools:

- Crystal Ball
- DEMOS
- @RISK
- STELLA
- VENSIM
- Time-Zero
- SCEM (DOE conceptual model builder)
- MATHEMATICA
- ERDAS-IMAGINE
- HSI modeling package (USFWS) (Habitat Suitability Index)

6. What can be done with modeling, simulation and analysis in this area? (Examples, success or non-success stories)

Discussion: Questions raised during the discussion included: Why don't widely-used "core" models for risk assessment exist as they do for other areas—such as dynamics of river systems. Why does everyone tend to develop their own site-specific or situation-specific models? One reason is that individual agencies prefer their own internally-developed models. A universal model to do everything would be cumbersome and unwieldy. Therefore, separate models to address specific aspects of a problem are developed. Models often are only used to look at "trends" or to make a quick decision, for which simplistic models may be adequate. Many models exist that describe ecosystem functioning (e.g., grasslands). These models can provide input to the risk assessment process, although they do not predict risk *per se*.

Use of models frequently seems to be arbitrary or after-the-fact. Ecological risk assessment seems to be an area in which model results tend not to be accepted. Radiological modeling results seem to be more accepted as compared to non-radiological situations. Air dispersion modeling also seems to be acceptable. Many geological situations are difficult to model. Results from most models potentially could be used in making decisions. Cost or regulators may drive the use of inappropriate models. There probably are more successful physical models in contrast to biological models. This undoubtedly is because biological systems are not well understood and therefore not conducive to modeling. There also are more data on physical systems. There is little funding for biological studies.

The team shared a few "success stories," where success was defined as when modeling results were used in decision-making or when results were accepted by peers. Examples of success include dose reconstruction projects, fisheries management, and RESRAD and air dispersion models. There probably are many local unpublicized success stories (e.g., wherever models are used to demonstrate compliance). An example of a probable non-success story was dioxins.

7. If modeling and simulation is not being used, or not being used successfully, why not?

Discussion: The team listed a number of reasons why models are not used:

- Lack of education, data, process knowledge, appropriate models, knowledge of which models to use, and universally-accepted models.
- Uncertainty
- Cost and scheduling
- Over-expectation (lack of ability to model)
- Models are often not understood (i.e., black boxes) and/or not easy to use
- Modeling is not prescribed (there are other alternatives)
- Lack of communication among modelers, with the public, with customers/clients, and with management.

8. Is there a gap between the development of models and simulation tools and methodologies and their application? Are new models, tools, and/or methodologies needed?

Discussion: The team gave a conditional "Yes" answer to this question. In some areas, development also is needed, and there is beginning to be some realization of this. There has to be recognition that appropriate models for the situation may or may not be available. Appropriate data also may not be available. Model development leads application development about a year. There is a lack of money (and acceptance) for model development.

Models have not been used in adaptive management situations. DOE has not been proactive in modeling development and application. There frequently is a lack of scheduling/lead time in realizing the necessity or desirability of model development. There is often disagreement on the algorithms to be used.

The gap between application and development is primarily caused by a lack of communication (e.g., there may be perfectly good models that nobody knows about). Another reason for the gap is that there are needs that require application but there are no models that are good enough (i.e., there needs to be more development).

9. Have there been cost/benefit studies for various models and simulation, and analysis tools and methodologies? Do we expect a good payoff if efforts are expanded into modeling and simulation?

Discussion: The team compared modeling to other alternatives. Modeling is less expensive than going out and doing the same thing in the real world. (Conversely, enough must be done in the real world to verify the modeling.) Models become much more cost-justifiable as the scale of the problem being investigated becomes increasingly larger, temporally and/or spatially. In the risk arena, there may be ways in which models can be used to reduce the need for engaging in day-today repetitive activities (e.g., data collection). Models can be used to identify areas that do not require cleanup. Models are cost effective if they reduce the cost of doing business and increase knowledge or understanding. While the team believed that there is a payoff, none of the participants could cite a specific cost/benefit study.

10. What modeling and simulation techniques are shared with other interest groups?

Discussion: Many analytical techniques are shared. DoD does some classified work. DoD and the entertainment industry spend large amounts of money on simulation techniques. Compatibility may be a problem. Physical models may be outputting information on a time scale that is inappropriate for input into an ecological model (e.g., emission output information at times when plant stomata are closed). Interfaces between models need to be carefully formulated.

11. What are the other benefits that can be obtained from modeling and simulation?

Discussion: The team listed other benefits as follows:

- Communication with public and decision-makers
- Understanding and knowledge
- Facilitating the decision-making process
- Testing assumptions and theories about systems
- Quantifying uncertainties
- Developing and formalizing conceptual models
- Quantifying analyses of alternatives, assumptions, etc.
- More effective policy development
- Human and environmental safety
- More businesslike approach to environmental management decisions at federal facilities
- Identifying research needs to address data gaps and lead to greater efficiency.
- Better targeting of scarce resources.

12. What measures can be used for assessing how well modeling, simulation, and analysis are being applied?

Discussion: Measures that could be used for assessment include:

- Frequency of (appropriate) use
- Cost reductions; better resource utilization and allocation
- Credibility/public acceptance
- Reflection of reality
- Number of experiments generated because of the use of the model

Conclusions

The following conclusions were reached following the workshop discussions.

· *Risk management is the new paradigm for federal facility operations.* This is the theme that ran throughout the Health and Ecological Effects I session. There was a consensus that risk is the appropriate measure for evaluating both human health and ecological impacts.

· *Human health and ecological systems are the drivers for risk management.* Because human health and ecological impacts are endpoints for decision making procedures, models of source term and physical transport must be designed to provide inputs to the human health and ecological models at the appropriate scales in time and space.

· *Human and ecological systems are complex and dynamic.* The design of models for these systems depends upon the temporal and spatial scale defined in the questions to be addressed. Human health and ecological models must be able to address multiple media, multiple contaminants, and multiple endpoints. For example, in human health assessments, questions are often posed for impacts at both the individual and population levels. In ecological assessments, both individual and population responses may be considered, but the question posed may be framed in terms of concentrations of contaminants in game animals, the likelihood of local extinction of populations, or the death of individuals of threatened and endangered species. Natural variability must be considered in these models. By natural variability, we mean to emphasize that there can be differences among populations of the same species, and certainly differences among individuals that need to be considered. We want to emphasize that natural variability is different from uncertainty that results from lack of knowledge; natural variability cannot be reduced by gathering more data, as is the case with uncertainty.

Appendix G. Health and Ecological Effects II

Health and Ecological Effects II Interest Area Team

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The initial goal of the team was to address the roles that modeling and simulation play in estimating the effects of the exposure of contaminants and stressors on humans and ecological receptors. The exposure could be to contaminants or to stressors not considered as being chemical or radiological contaminants. The team identified six types of situations or problems that could be addressed by modeling and simulations:

(1) The amount of hazardous material that reaches receptors

(2) The duration of exposure

(3) An estimate of the magnitude of adverse effects to receptors

(4) The provision of risk communications tools

(5) A means to support decisions and foster environmental stewardship

(6) A means to quantify the uncertainty of estimates, and/or identify the sensitivity of models.

Modeling developed or applied in support of user-generated problems suggests a variety of user/client communities: the public or different subsets of the public; regulators charged with writing and enforcing relevant legislation; scientists and analysts who develop and maintain different models; and owners and operators of facilities that are affected by the processes being modeled or who are required to comply with different environmental regulations and orders.

The team identified six prototypical problems/situations:

1. New products/industrial systems
2. Brownfields Redevelopment

3. Land Management
4. Facilities Compliance and Single versus Multiple Regulations
5. Environmental Restoration/Installation Restoration
6. Emergency Response

For each of these areas, the teams focused on several themes: the approach should not be limited to just contaminants; an ecosystem analysis is important; market-based approaches should be used; and multimedia permitting should be considered. The paragraphs that follow highlight the chief points captured during the discussions of these six areas.

(1) New Products/Industrial Systems

- Constraints
- Rate-based versus absolute
- Minimization/substitution issues
- Cost/benefit
- Information confidentiality
- “Approved set” of models
- Variables
- Compliance (cradle to grave)
- Geological climate context models
- Manufacturing processes (and alternatives)
- Emissions
- Air
- Water
- Wastes
- Thermal
- Noise
- Radiation
- Fate/transport
- Exposure and risk
- Resource consumption
- Transportation
- Cost/benefit

Exposure Model

- Credible input parameter
- Distributions
- Interdependence relationships
- Site specific data

- Exposure concentration versus ambient (micro-environments)
- Bio-availability (general sense) models
- Utilization of bio-markers development
- Indicator species
- Sentinel species
- Hindcasting
- Alternative endpoint models
- Continuous modeling with data collection (interactive-iterative)

Hazard Model

- Better integration
- Better modeling of agent interactions
- Data?
- SAR
- Continuous versus yes/no hazards
- Address greater endpoint specificity
- Effect specific hazard models
- Eco-interlevel extrapolations assessment
- Endpoints, measurement endpoints
- Effect relevance
- PBPK models
- Mechanistic models
- Assessment of repair/detox
- Replacement of R&D as a concept
- Small population hazards
- Alternative endpoints
- Effect severity

Communication and Organization Issues

- Increased GIS application to all spatial problems
- Better match of models to data
- Better communication
- Need to ensure data interchangeability
- Better approaches to capture data from small communities
- Descriptive versus predictive
- Better communication of full scope of uncertainty
- Quantitative and qualitative tools for visualization
- Defining the nature of uncertainty
- Input on decision process

- Value tradeoffs in multi-dimensional decision space
- Stakeholder of manipulation of models and information

Risk Characterization

- Alternative endpoint models
- Non-contaminant stressors
- Habitat loss
- Fragmentation
- Degradation
- Community disruptions
- Indirect effects
- Population/community models
- Loss of spatial information
- Practice versus possibility
- Choice of target (who?)
- Combination of exposure distributions with hazard distributions
- Fuzzy uncertainty
- Competing risks

Key Dialog Areas

- Fate and transport
- Temporal/spatial variability
- Bio-accumulation and bio-magnification
- Next workshop needs more media, especially indoor air exposure media
- Transformation (in different media)
- Natural attenuation
- Spatial data input uncertainty
- Better communication of sources of uncertainty
- Study of model versus perimeter uncertainty

(2) Brownfields Redevelopment

- Constraints
- Broad public involvement
- Land location/condition
- Cost/benefit and risk/benefit
- Variables
- Government economic support
- Pending legislation (EPA program)

- Models
- Off-site source contributions
- RBCA
- Population exposure
- See also New Products/Industrial Systems

(3) Land Management

- Constraints
- Unique regulatory context
- Mission-driven
- Ecosystem management
- Variables
- Spatial context
- Ecosystem, political, special
- Adjacent landowners
- Models
- Land use
- Cumulative effects
- Conservation
- Cultural
- Biological
- Mitigation/replacement
- See also New Products/Industrial Systems

Cumulative Effects

- Non-contaminants that affect land and ecosystems
- Economic
- Noise

Mitigation/Replacement

- Better equivalency models clearly exist
- Incorporate stakeholder values
- Better hydrologic models for wetland replacement

Land Use Measures

- Contaminants (see above)
- Cumulative non-containment
- Better location-specific economic effects

- Longer term perspective

(4) Facilities Compliance and Single versus Multiple Requirements

- Constraints
- Unique regulatory compliance
- Enforceable federal agency requirements/exemptions
- Citizens
- Information confidentiality
- “Approved set” of models
- Regulatory imprecision
- Variables
- Unique activities for federal
- Monitoring data richness
- Upcoming “credible evidence”
- Models
- Models of unique activity
- See also New Products/Industrial Systems, Brownfields Redevelopment, and Land Management

(5) Environmental Restoration/Installation Restoration

- Constraints
- Unique regulatory context (FFCA multiparty)
- CERCLA/SARA/RCRA
- Natural resource damage assessment
- Funding and cost/benefit
- Time frame
- Removal/disposal restriction
- Unique hazards (including worker health)
- Variables
- Historical data quality
- Population density/proximity
- Political division (variable state and regional programs)
- Models
- Fate and transport (retro and prospective)
- Exposure, hazard, risk (see New Products/Industrial Systems)
- Multistressor
- Multi-endpoint
- Multimedia is usual rather than innovative
- Natural attenuation

- Non-contaminant effects of remediation
- Watershed (see Land Management)
- Health studies

Public Health Assessments

- Better models for data selection
- Practice versus available methods
- Population choice
- Reflection of values

(6) Emergency Response

- Constraints
- Real-time with time course
- Short response time
- Very high public visibility
- Polarized public
- Training/expertise needs
- Limited data
- Limited response options; variables
- Agents
- Environments
- Infrastructure
- Transportation, medical, equipment; variables
- Communication
- Internal
- Public education and response
- Human factors (reactions change situation in real time)
- Models
- Key characteristics
- Easy to use
- Portable – broadcastable
- Cheap
- Hazmat control and response
- Planning and simulation

Emergency Response Models

- Better distribution (before, during)
- Perceived inadequate parameters (before, during)
- Better stakeholder ownership (before, during)

- Extreme sensitivity to *local* conditions/human factors (before, during)
- Need real-time feedback with all factors (see sample/model interactions) (during)
- On-the-fly contingency response (during)

Exotic Species (e.g., zebra mussels, gypsy moth, hanta)

- Constraints
- Unique transmission pathways
- Variables
- Models
- Epidemiology/pathogen models
- Ecological models (see Land Management)
- See Emergency Response and other problem areas

Appendix H. Infrastructure

Infrastructure Interest Area Team

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The Infrastructure interest area team considered its vision with respect to the infrastructure of modeling, simulation, and analysis (MS&A) for environmental management and came up with: "*Better Decisions through Better Analysis through Better Modeling and Simulations*." It also developed a goal: "*Provide better support for Environmental Management (EM) policy decisions that lead to resource allocations*." The team devoted roughly equal time to two topics: (1) the modeling of infrastructure, and (2) the infrastructure of modeling. The first infrastructure category comprised any and all of the equipment, facilities, networks, people, organizations, processes, etc., required to accomplish the objectives of environmental management (EM), including the infrastructure required to support just the MS&A to accomplish those objectives. The second topic focused on just the MS&A infrastructure for the three agencies with EM responsibilities represented at this workshop, but was believed to be generally applicable for MS&A within other agencies with significant EM responsibilities.

The terms ***modeling, simulation, and analysis*** denote the following:

- Modeling—the construction of conceptual, descriptive, mathematical (including logical), or combined representations of the characteristics and behavior of equipment, facilities, networks, people, organizations, and processes.
- Simulation—performing the calculations on the values of inputs (e.g., the numerical values of parameters and the specification of any branching or choices that must be made) using the mathematical representation of the model to provide the desired results. When mathematical models are involved, the results may be numerical or in the form of descriptive material or recommendations.
- Analysis—the interpretation of the results, and their implications, of the calculations and simulations for mathematical models or the implications of conceptual and/or descriptive models.

Many scientists, engineers, and mathematicians apply the term ***modeling*** to all of the above and refer to themselves as modelers. Some prefer to restrict the use of the term ***simulation*** to the simulation of dynamic systems where characteristics change with time. Many investigators apply the term ***analysis*** to the definition of analysis given above, as well as to the simulation activities given above when only calculations for static systems are involved.

Every decision maker uses models in making decisions, even if they are only informal, approximate, undocumented, and even poorly formulated conceptual models contained in the decision maker's mind and of which the decision maker may not even be consciously aware. The emphasis here is on formal models, including simulation and analysis tools, ranging from conceptual and/or descriptive models through approximate models and higher-level models to often very detailed, relatively accurate models.

- *Conceptual and/or descriptive* models may be approximate, but are at least well-understood, as well-formulated as feasible, and well-documented, including descriptions of all recognized gaps. In these models, the emphasis is on analysis rather than calculation or simulation. For example, these models are used to estimate the significance of results, uncertainties, and risks in areas that are often relatively straightforward. They require little in the way of human and physical resources.

- *Approximate* models are used for obtaining results of accuracy appropriate for limited purposes; e.g., establishing the significance of various factors, illuminating general principles, and providing order-of-magnitude estimates, all of which may be useful in decision making. These models are well-understood; are as well-formulated as feasible; are well-documented, especially with respect to known gaps, the approximations involved, and the solution algorithms; and are thoroughly validated. They provide values for measures of uncertainty and risk where possible. Because they require only modest human and physical resources for their application, they may be particularly useful for higher level decision makers who want to perform their own MS&A. This would enable the decision makers to obtain results more quickly when needed with little advance notice and to address their specific needs more efficiently. For example, such models would permit exploration and answers to "What if?" questions.

- *Higher-level* models typically address broad issues involved in decision making or overall results for complex systems, perhaps by applying approximations or summarizing and integrating the results obtained from more detailed MS&A. They involve calculations and simulations, necessitating the use of more or less modest human and physical resources. If sufficiently user-friendly user interfaces are provided, it may be feasible for decision makers themselves to personally perform some or much MS&A using the models to reduce the time required to obtain results required on short notice and to address their specific needs efficiently. The results of higher-level models are relatively easily understood in general, with only modest subsequent analysis being required, although they may exhibit emergent behavior when complex systems are being modeled. Generally, these models are well-formulated with few or no gaps. The model itself, including all subsidiary models, databases, assumptions, uncertainties, gaps, etc., is well documented and validated insofar as possible or reasonable, along with the algorithms used to produce results.

- *Very detailed models* are relatively accurate rather than approximate, specialized or comprehensive, relatively complete with few or no gaps, well-formulated mathematical models. All submodels, in addition to the principal model, databases, assumptions, uncertainties, approximations, and solution algorithms, are well documented and validated as far as possible or reasonable. Substantial financial, human, and physical resources may be required to perform calculations, and considerable expertise may be necessary for the evaluation and interpretation of results and the placing of these results into forms that are useful to decision makers.

Prior to the workshop, several lists were prepared to provide a means for efficiently starting the Infrastructure interest area discussions. These lists are shown in Tables H-1 through H-3. Table H-1 lists examples of various kinds of infrastructure required to support EM within the DOE, DoD, EPA, and other government agencies. Table H-2 lists examples of the scales, scopes, and time frames for which MS&A has been, and is being, performed to support the EM infrastructure-related activities of such agencies. Table H-3 is a more detailed list of examples of topics for environmental MS&A being addressed to support EM. Note that the three extensive lists are not necessarily complete.

Table H-1. Kinds of infrastructure required to support EM

Transportation Networks & Equipment & Waste Packaging & Handling Equipment	Temporary & Permanent Waste Storage & Disposal Facilities & Equipment	Processing & Manufacturing Equipment, Systems & Facilities
Roadway Railway Pipeline Water Air Vehicles & packaging & handling equipment	Containment structures Monitoring systems Packaging, handling, etc. Equipment	Packaging fabrication Waste treatment Contaminated site remediation
Communications & Data Systems	**Special Structures**	**Scarce Resources That Must Be Well Managed to Achieve Cost Effectiveness**
Data processing & transmission Monitoring Security Signals, alarms, etc. Ordinary & emergency communications	Contaminated buildings Containment Hot cells & laboratories Special-purpose buildings	Special materials Management skills Trained personnel Technical expertise Special equipment Special facilities

Table H-1. Kinds of infrastructure required to support EM (continued)

Utilities Production & Delivery Systems	Special Equipment	Processes & Activities That Support EM

Electricity Gaseous fuels Liquid fuels Fire protection Sewers and drains Water Steam HVAC Compressed air Breathing air	Robotics Transfer piping systems, tank farms, etc. Analysis, monitoring, etc., capabilities Mobile & modular equipment	Business processes Privatization Design & engineering Construction Operations & maintenance Decontamination, decommissioning & closure Landlord functions Sampling & site characterization Program, project, facility, site, etc., management Environmental, health & safety, regulatory, financial, legal, stakeholder involvement, etc. Research, development, demonstration, testing, & evaluation (RDDT&E) Modeling, simulation, & analysis to support all of the above

Table H-2. Kinds of scopes, scales, and time frames supported by MS&A in the EM infrastructure.

Scopes Scales, and Time Frames
Individual pieces of equipment, structures, etc.
Entire process trains & manufacturing lines
Single-purpose & multipurpose facilities
Large complex sites
Sitewide, local, regional, & national networks
Entire DOE Complex
Individual activities, steps, & phases
Entire processes
Entire life cycles
Temporary & permanent
Public & private sector infrastructure
With & without treating all externalities
Resources used at more than one site
Long, complex, multistage, and/or multisite activities, processes, remediations, projects, programs, etc.
Government issues at various levels (e.g., federal department or agency, environmental management department, individual site, individual facility)
Contractor issues

Table H-3. Kinds of specific systems and activities subjected to MS&A.

Systems and Activities	
· Program and project management	· Decision support

- Engineering & design
- Requirements & functionality analysis
- Reliability, availability, & plant factor
- Manability
- Operations & maintenance
- Monitoring
- Communications
- Chemicals & supplies
- Equipment
- Process trains & manufacturing lines
- Facilities
- Transportation equipment
- Software development
- Facilities & sites
- Complexes & networks
- Startup & shutdown
- Contracting
- Packaging, handling, & shipping
- Cost estimating
- Cost//benefit/effectiveness
- Finance
- Human health & safety impacts & risks
- Human factors
- Training
- Societal values
- Site characterization
- Environmental impacts
- Secondary wastes
- Emissions reduction
- Business processes
- Commercialization
- Contaminated site remediation
- Resources utilization
- Systems engineering & analysis
- Supportability, operability, & maintainability
- Manufacturability or produceability
- Construction scheduling & management
- Utilities (e.g., energy, water)
- Vulnerability & security
- Data processing & transmission
- Spares & repair parts requirements
- Activities & processes
- Structures
- Transportation networks (e.g., roadways)
- Waste handling & packaging equipment
- RDDT&E
- Process trains & manufacturing lines
- Deployment
- Mobilization & demobilization
- Marketing & sales
- Modernization, upgrading, & expansion
- Financial risk
- Economics
- Budgeting
- Technical risk
- Staffing
- Regulatory
- Societal impacts
- Stakeholder communications & involvement
- Air, soil, water, etc., fate & transport
- Energy efficiency
- Climate change
- Privatization
- Landlord functions
- Decommissioning, decommissioning & closure
- Scheduling & routing
- Chemical analysis, radioactivity assaying, etc.

Most MS&A, without which not much can be accomplished, or at least not efficiently, accurately, and cost effectively, is performed for such systems and activities by private-sector contractors, rather than by the government agencies, who have contracted for the design and construction of facilities (e.g., for the treatment, storage, and final disposition of wastes; their operation and maintenance; or contaminated site remediation). In addition, agency employees or independent consultants or consulting firms have performed and continue to perform EM infrastructure-related MS&A to support decision making within these agencies. Much of this MS&A is performed as a matter of course, but the point is that someone must ensure that these activities are done adequately. In addition, government decision makers should determine who should perform these various kinds of activities and how much MS&A should be done. The performers might be the private sector, government agencies, and/or independent consultants.

The team could not address, in the allotted time, all of the many infrastructure categories and topics listed in Tables H-1 through H-3, but instead considered a few general categories and topics. The team identified four broad categories of infrastructure as being of particular importance in general and specifically for the three agencies with extensive EM responsibilities that were represented at the workshop. The criteria used in assessing importance included complexity with respect to the decisions to be made and the total economic impacts and impacts on health, safety, society, and the environment. These four categories were:

(1) The processing of radioactive, chemical, and biological wastes to render them innocuous or convert them to forms suitable for interim storage or ultimate disposal, and the cleanup of sites contaminated with such wastes.

(2) Transportation in general because of the emissions, including toxic wastes (e.g., sulfur and nitrogen oxides and particulates) and greenhouse gases (e.g., carbon dioxide from roadway vehicles, railroad engines, watercraft, and aircraft fueled by fossil energy); leaks of fuels during delivery and use; and the transportation of radioactive, chemical, and biological wastes, including packaging and handling, in particular.

(3) The interim storage and final disposition of radioactive, chemical, and biological wastes.

(4) Electric power production fired by fossil fuels because of emissions from generating units, including toxic wastes and greenhouse gases.

Expert Systems

One of the present concerns of the management of the DOE and other federal agencies is the preservation of the knowledge base represented by the expertise of their own employees and those of their consultants and contractors. Government agencies have invested large sums of the public's tax money for the development of much information of lasting value that has not been recorded anywhere. Much of this information is in danger of being irretrievably lost as a consequence of the changes in duties or employment, incapacitation, or death of personnel. The team felt that there is a responsibility to capture and preserve such data. To some extent, models constitute repositories of this kind of valuable information. One way to capture and preserve such information is through the construction of expert systems. The knowledge of more than one expert can be encompassed in one expert system. In addition to helping preserving "corporate knowledge," expert systems offer numerous other benefits, which were discussed by the team. Well-designed expert systems do not have gaps in their knowledge base. They do not ignore important aspects of a problem, or make mistakes due to the press of time.

It appears that the greatest successes with expert systems are achieved when one or more of the following is met:

- The problems addressed by the expert system are difficult, but the topic is of modest scope and well understood, the theory is well established, and the knowledge base is adequate.

- The knowledge base incorporated in the data base is so extensive that recall of all of the data necessary to solve important problems is difficult for an individual, or even a group, whether the problem itself is particularly difficult or not.

- The treatment of a large class of problems can be generalized so that the cost of development of the expert system is far outweighed by even modest improvements in solving problems using an expert system.

- The time permitted for obtaining a recommendation is so short that consultations with experts are not feasible. An example is the case of expert systems that aid in responding to emergencies, such as natural disasters, military actions, terrorist acts, and catastrophic failures of process equipment or containment of hazardous materials.

Numerous relatively mature commercial tools exist that incorporate and facilitate the application of the best techniques for constructing good expert systems efficiently and for eliciting information from experts effectively.

Improving Communications

The comment frequently has been made that the MS&A community should work harder to communicate effectively with decision makers. The most common view is that decision makers need to be made more aware of the value of various kinds of MS&A; the products that can be expected; how rapidly various kinds of products can be delivered; and the resources required. The emphasis is on educating decision makers; however, this is a two-way street. The MS&A community also must make a greater effort to determine what, at a minimum, decision makers really need and what they would like to obtain from MS&A in addition to satisfying their minimum requirements. Decision makers can help make this process easier by also providing education in these areas to the MS&A community.

The team discussed benefits that might be achieved as a result of enhanced two-way communication of this type. It can allow the MS&A community to more accurately and efficiently address the needs and desires of decision makers. An important goal of MS&A is the development of at least an adequate understanding of the risks (e.g., financial, human health and safety, and environmental) involved in making a decision. This is the first necessity for effective risk management and risk reduction, which are follow-on goals of much MS&A. Therefore, knowledge of the risk preferences of decision makers can help the MS&A community target their efforts more accurately.

Decision makers can be risk averse. They may prefer decisions that maximize the probability associated with outcomes with desirable results and perhaps reduce the range of possible outcomes, possibly at the expense of not being able to obtain the greatest possible rewards or even a lower expected result as it is known. They can also be risk takers. They may be willing to consider a wider range of outcomes and risk losses in order to achieve maximum results. Other decision makers may be risk neutral. They may make decisions based strictly on expected outcomes as far as they are known. The products of the MS&A community should be tailored to the risk preferences of the decision makers whenever feasible and reasonable.

Both decision makers and the MS&A community must recognize that the perception of significant uncertainty (one definition of risk) is subjective. Uncertainty perceptions derive in part from individual preferences, while risk can be subjective or objective. Objective risks are ones for which the occurrence of possible outcomes is uncertain and the probabilities of occurrence associated with the various outcomes are known relatively accurately. The values of the probabilities are generally not in dispute as a result of the availability of adequate theory or experimental data. A simple example of an objective risk is the flipping of a fair coin, or at least one for which the bias has been accurately established. Clearly, MS&A can assist in the evaluation of objective risks.

Subjective risk arises when there is no adequate theory or database of experimental results to provide relatively undisputed accurate values for the probabilities of possible outcomes. The quantification of subjective risk is usually based on the experience of decision makers or consulted experts, but even here MS&A can aid in the efficient and accurate elicitation of information that can help quantify subjective risk.

Another topic discussed by the team was improvement in the packaging of MS&A results: what the MS&A community can do to improve the communication of their products and their use by decision makers. First, of course, it is necessary to ascertain the desires of decision makers in these areas. They may be different for different decision makers and may have to be individually determined and addressed.

At a minimum, MS&A efforts must be honest and provide products that are of adequate accuracy and completeness, must include measures of uncertainty, and should be understandable and believable. Perhaps the most important aspects of believability are providing convincing evidence that the information available for examining all significant relevant factors is adequate, that the relevant factors have been addressed in an acceptably accurate fashion, and that unexpected, especially counterintuitive, results are satisfactorily explained.

The results of an MS&A effort, especially when the results are complex and require extensive interpretation, are much more likely to be immediately useful and used when they are provided to decision makers in a polished form and are appropriately condensed. The results should be condensed where feasible and with all the necessary interpretation, including quantification, or at least adequate discussion of the risks and uncertainties involved. If the results are presented in a quality briefing package, decision makers can use this to brief their superiors in the management hierarchy on the basis for their decisions. Most decision makers would find this highly satisfactory and very welcome.

Decision makers may request and be provided with MS&A tools that they can use themselves to obtain results quickly when time is short, explore possibilities by addressing “What if?” questions, and generate results targeted specifically to immediate concerns and personal preferences. These tools might be based on the *conceptual*, *approximate*, and *higher-level models* previously discussed. In such cases, it is clearly important that the design of the user interface facilitates use by persons relatively unfamiliar with the MS&A tool. Casual users generally welcome MS&A

tools that can produce attractive and sophisticated presentation materials and useful reports with a high degree of automation. This is an area where expert systems that help users solve their problems efficiently through use of the tool can be very useful. Such expert systems, which are often simple, crude, and minimally effective but becoming increasingly sophisticated and useful, are often referred to as *wizards*, and are being provided as part of many software packages to supplement more traditional help files and online documentation.

If such tools can be constructed using software that is more or less familiar to decision makers (e.g., constructed and applied using spreadsheets dominant in the marketplace and widely used applications packages) the tools are more likely to be readily used by the decision makers. Because the decision makers may already possess the basic software and the hardware required to apply the tools, the added investment in software and hardware is perhaps minimal. Also, the decision makers will already be experienced in at least some of the operations required to apply the tools.

There is a wide variety of powerful, economical, user-friendly, widely used, mature commercial software for such tasks as risk analysis, cost and economic modeling and simulation, and decision-support. This software is available as add-ons to spreadsheet packages. A particularly powerful example of such software is *decision-tree* add-ons that can (1) apply utility function methodologies, (2) use other spreadsheet add-ons to perform cost calculations, Monte Carlo risk analysis, and other computations to provide input to decision-trees, and (3) generate reports and graphics to document and illustrate recommended choices, estimated costs, utilities, risks, and other quantities of interest. Such tools often appear to provide exactly the level of MS&A that is especially useful for many decision makers.

The team proposed several MS&A infrastructure options for improving the two-way communications between decision makers and the MS&A community, and it was suggested that DOE could take the lead in developing such MS&A infrastructure.

- Assisting decision makers in acquiring hands-on experience in the running of calculations and simulations and in the interpretation of the results that are produced with various objectives where appropriate. This assistance could be through one-on-one interactions and/or workshops. It would enable decision makers to understand what is required to obtain meaningful results, how to use them, and/or how to obtain their own results on a more or less routine basis.

- Establishing an interagency MS&A working group to coordinate MS&A activities and interactions with decision makers, establish and maintain critical databases, ensure the establishment and maintenance of other importance resources, ensure that MS&A infrastructure once developed does not disappear without a trace, promote where feasible the transfer of government-funded MS&A products to the private sector, translate MS&A results for decision makers, and/or generally champion MS&A within and across agency and department boundaries.

- Creating separate intra-agency and/or inter-departmental organizations (working groups or individuals) that would accomplish the same objectives within various agencies or departments and/or across department and agency boundaries.

The team concluded that decision making can be made more efficient by using infrastructure system models, methodologies, and tools that address the complete life cycles and integrate all important internal factors and externalities. These factors include ES&H impacts, political, institutional, social, and other human behavior, as well as performance and costs, as discussed previously in the description of *higher-level models*. Such models could largely eliminate the necessity for assembling MS&A results that address various parts of the overall problem from disparate sources; the separate evaluation and winnowing required to select and assemble only the information required from each source; the possibility of failing to capture the effects of important interactions between individual parts of the total problem and detect possible emergent behavior; and the labor involved in integrating the constituent parts to address the overall problem. Without such an approach, hands-on MS&A for complex problems by many decision makers is virtually impossible.

Complex Systems and Systems Engineering

Complex systems, including much infrastructure, the infrastructure for complex MS&A, and individual MS&A tools, may be difficult to design satisfactorily. These systems may exhibit *emergent behavior*—behavior that might not be anticipated by considering the component parts of the system individually. Systems engineering (SE) methodology was originally conceived under the aegis of the DoD to counteract difficulties encountered in the design of complex weapons systems. SE is a methodology developed for the effective, efficient management of the design of complex systems. It is beginning to be applied to the design of complex DOE, DoD, and other government agency systems for manufacturing, environmental restoration, waste treatment, minimization, storage and disposal, etc. Applications include hardware systems, facilities, infrastructure, organizations, activities, and business processes. DOE, DoD, and other agencies have been attempting extensive reengineering, including privatization, of many of their activities and business processes in recent years with some successes, but in other instances have encountered severe difficulties which could be resolved using SE and other MS&A.

Increased emphasis in SE has recently been placed on such considerations as:

- Customer and other stakeholder requirements and desires for involvement
- Human health and safety
- Protection of the environment and sustainability
- Life-cycle costs versus benefits for very long lived, expensive, and complex enterprises, such as some environmental remediation projects
- The desire to treat all internal factors and externalities, including various aspects of human behavior

- Greater efficiency, quality, and cost effectiveness.

With the focus on these considerations, SE has come to encompass interactions with other systems external to the system being designed, in addition to the traditional design of equipment and facilities more or less in isolation, and the design for all phases of their life cycles. Relevant systems external to the systems to be designed may include various societal systems, such as the public, management, operating and maintenance crews, government, regulatory bodies, and other stakeholder organizations, the environment, and artificial physical systems. The phases of the complete life cycle of a system typically include implementation, operations, support, and ultimate disposal. The methodology of SE is also being applied to a greater or lesser extent in the development of complex new software packages, including software for MS&A (e.g., under the appellation of computer aided software engineering).

For sufficiently complex systems, SE can involve all of the traditional scientific and engineering disciplines and methodologies that support design, construction, and management, including MS&A of natural and artificial physical, biological, governmental, business, economic, and social systems. SE also involves some special extensions to established MS&A management methodologies and tools, especially with respect to controlling the design process; maintaining accountability and traceability; establishing requirements; determining the required functionality architecture; defining and designing interfaces between system subsytems and individual elements; and testing and verification.

The importance of establishing a set of requirements that is complete, feasible, and acceptable to all stakeholders is discussed throughout this report. Figures H-1 through H-8 illustrate various aspects of SE that are discussed in more detail following the figures. Figures H-9 and H-10 illustrate the importance of beginning to apply SE principles early in the life of a design project.

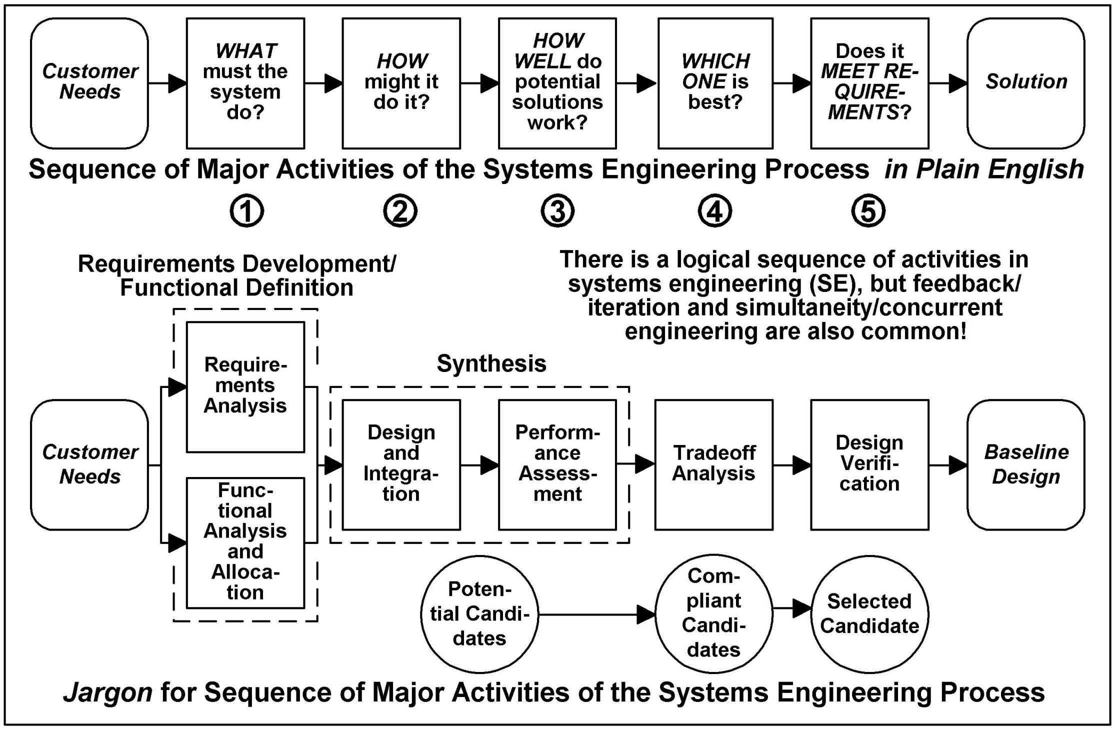

Figure H-1. Overview of systems engineering methodology.

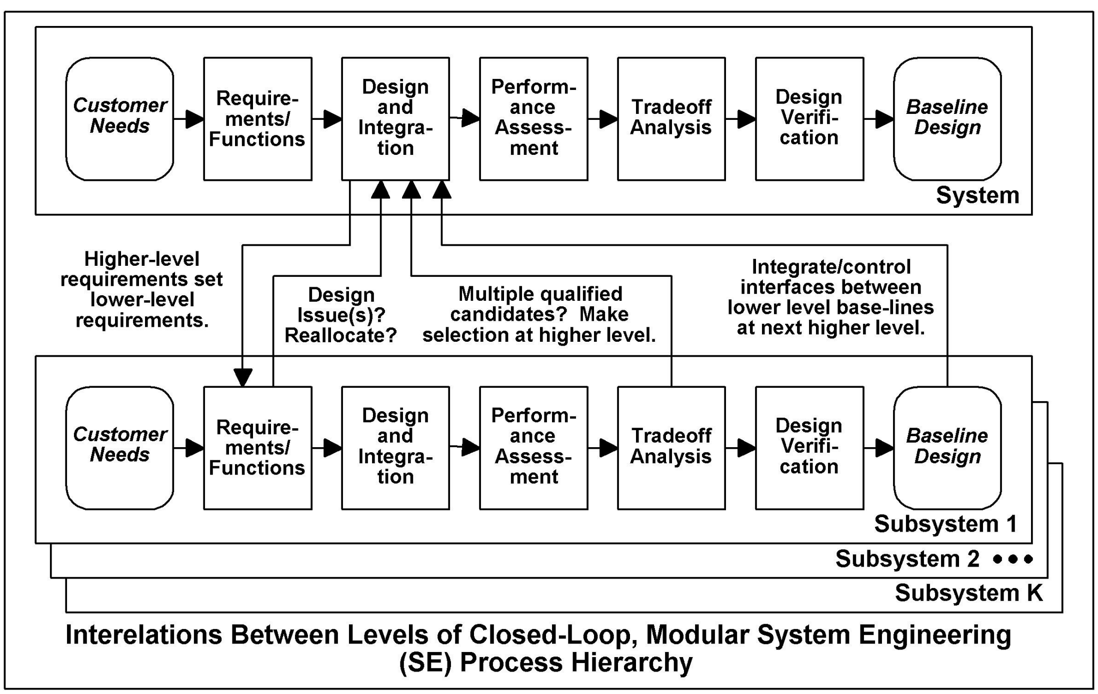

Figure H-2. Similar systems engineering steps are applied as necessary at all levels of the hierarchy of complex systems, with requirements flowing downward and interfaces, issues, and candidate selection upward.

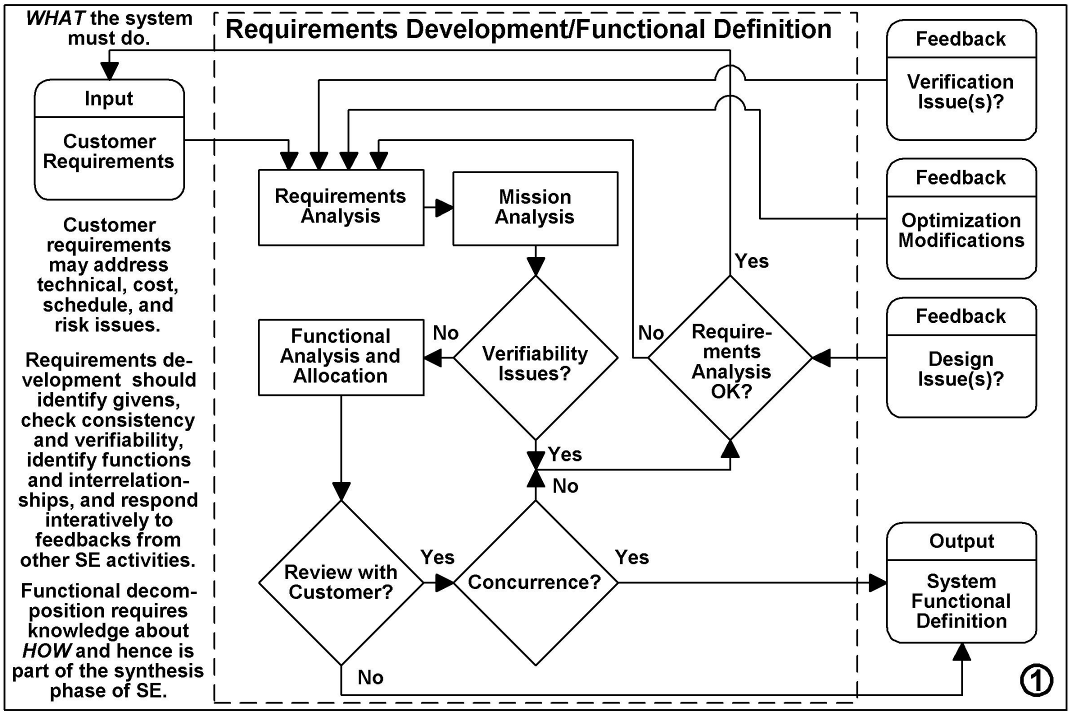

Figure H-3. A more detailed view of requirements and functional analysis activities of systems engineering.

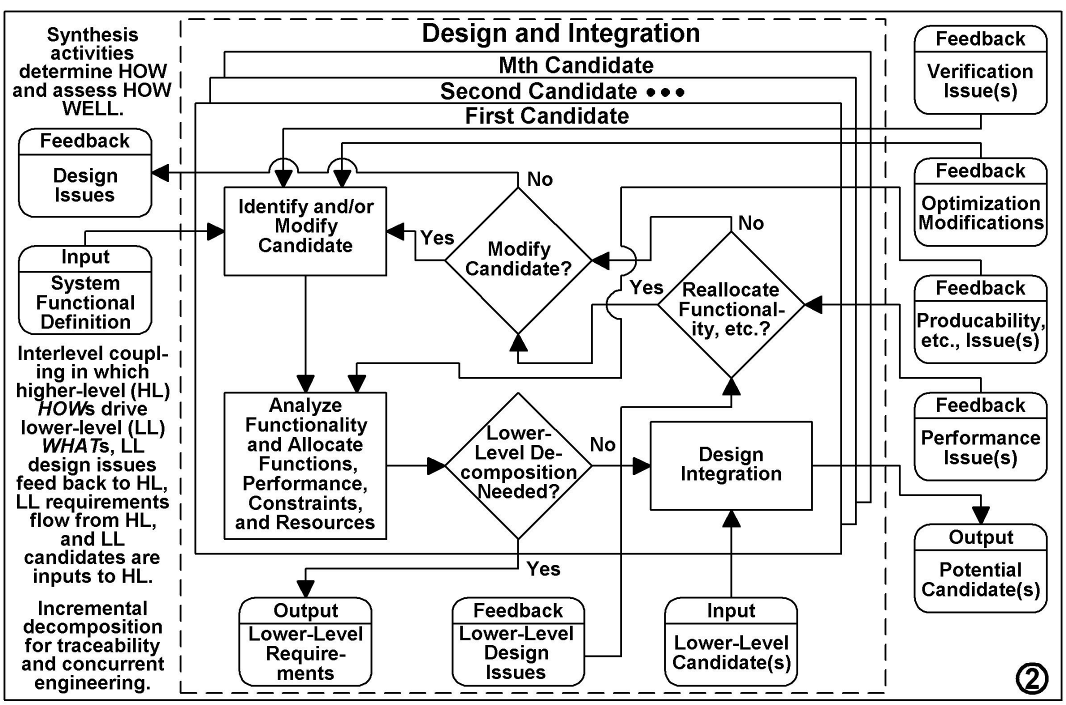

Figure H-4. A more detailed view of design and integration activities of systems engineering.

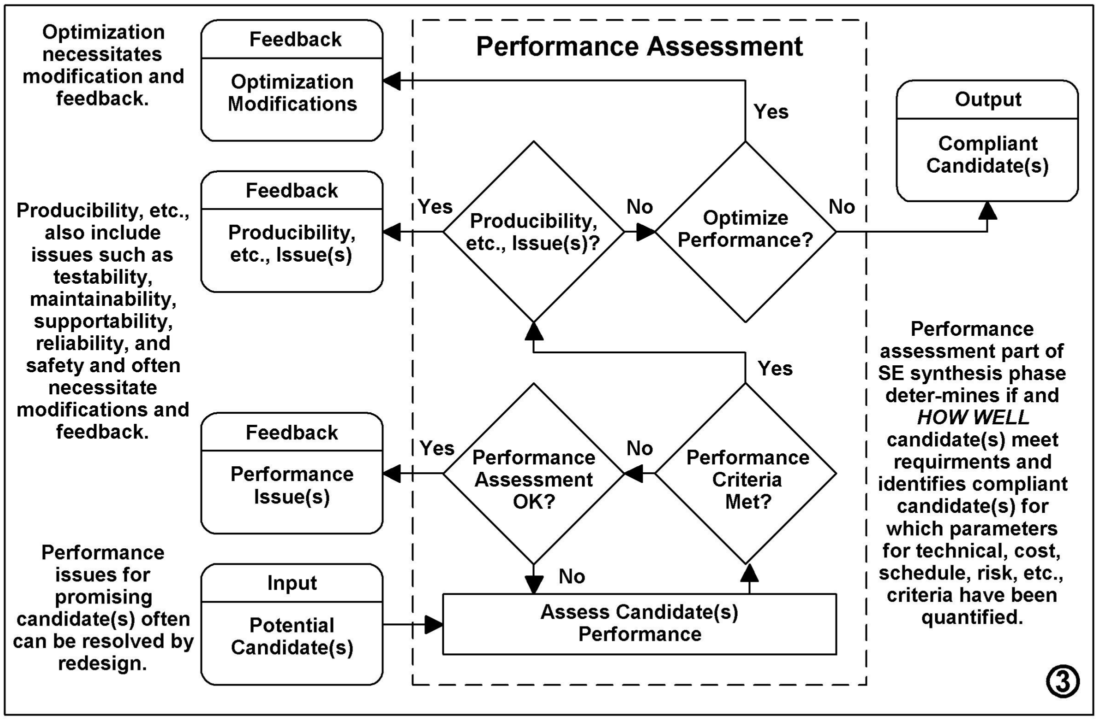

Figure H-5. A more detailed view of performance (including cost) assessment activities of systems engineering.

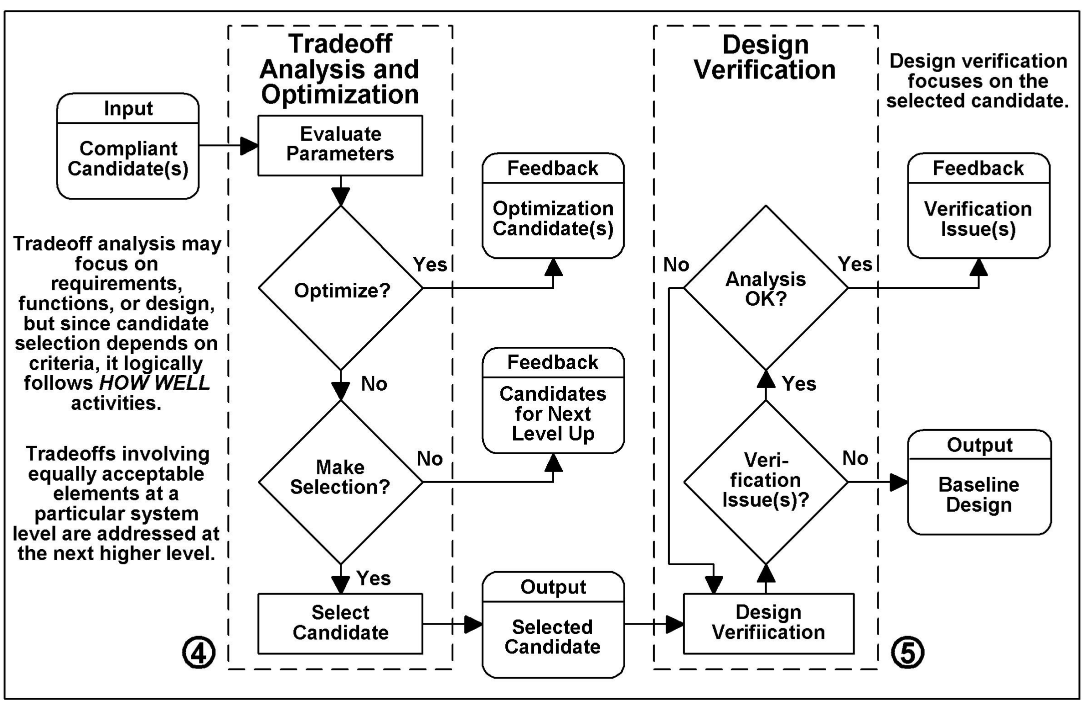

Figure H-6. A more detailed view of tradeoff analysis and optimization and design verification activities of systems engineering.

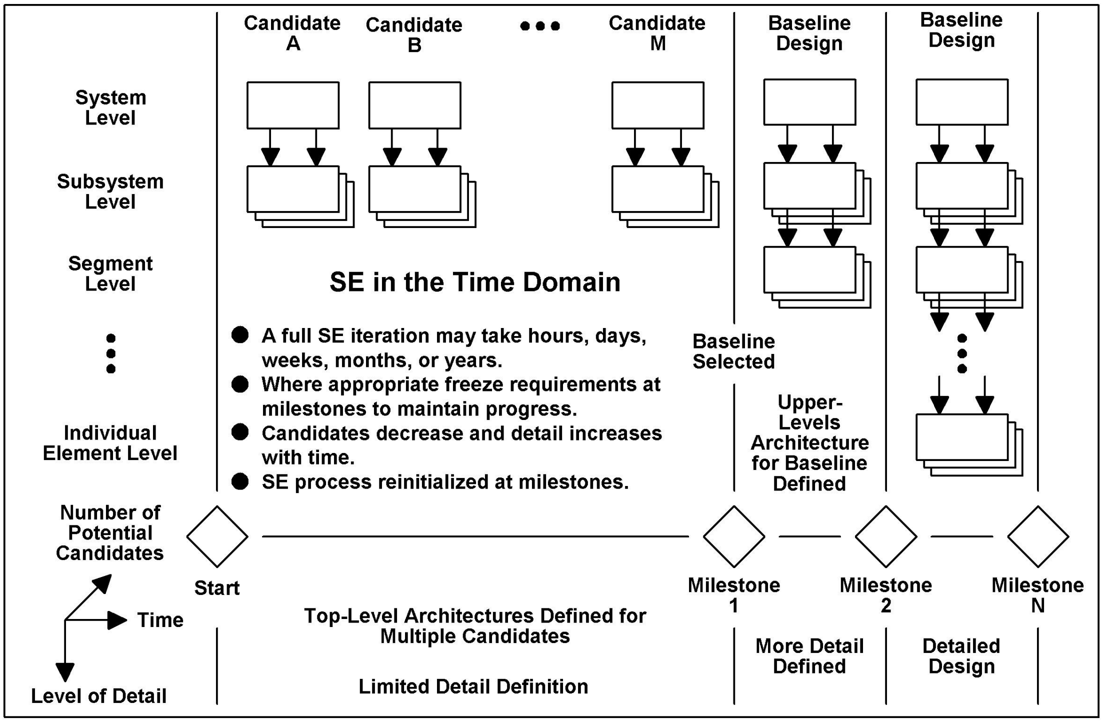

Figure H-7. The evolution of a systems engineering project through time.

Classes of Elements

Completion Criteria
Component
Constraint
Critical Issue
Decision
Domain Set
Engineer
Function
Interface
Item
Link
Originating Requirement
Performance Index
Responsible
Organization
Risk
Source Document
System
Test Configuration
Test Procedure
Verification document
Verification Event
Verification Method
User-Defined*

Attributes

Abbreviation
Alternatives
Assumptions
Capacity
Capacity Units
Choice
Component Type
Creation Date
Creator
Delay
Delay Units
Description
Document Number
Duration
Duration Units
Event Window End
Event Window Start
Exit Probability
Exit Type
Government Category
Item Type
Item Number
Event Duration
Mission
Mitigation Plan
Mitigation Status
Modification Date
Modification Time
Non-Government Category
Number
Other Paragraph
Paragraph Number
Paragraph Title
Priority
Problem
Protocol
Risk Factor
Risk Type
Size
Source Type
Technique
Units
Verification Level
Verification Status
User Defined*

* As Needed

Relationships & Inverse Relationships

Allocated To (Performs)
Built From (Built In)
Carries (Carried By)
Causes ('Caused By)
Comprised Of (Comprises)
Conducts (Conducted By)
Configuration For (Uses Configuration)
Connected To (Connects To)
Constrained By (Constrains)
Decomposed By (Decomposes)
Defines (Defined By)
Documented By (Documents)
Exhibits (Exhibited By)
Exits By (Exit For)
Forms (Formed By)
Generates (Generated By)
Incorporates (Incorporated In)
Inputs (Is Input To)
Is Associated With (Affiliates)
Is Basis Of (Is Based On)
Outputs (Output From)
Owned By (Owns)
Resolves (Is Resolved By)
Satisfies (Is Satisfied By)
Is Serviced By (Services)
Traces From (Traces To)
Verified By (Verifies)
User-Defined*

Figure H-8. Examples of items in entity-relationship-attribute (ERA) schema for systems engineering.

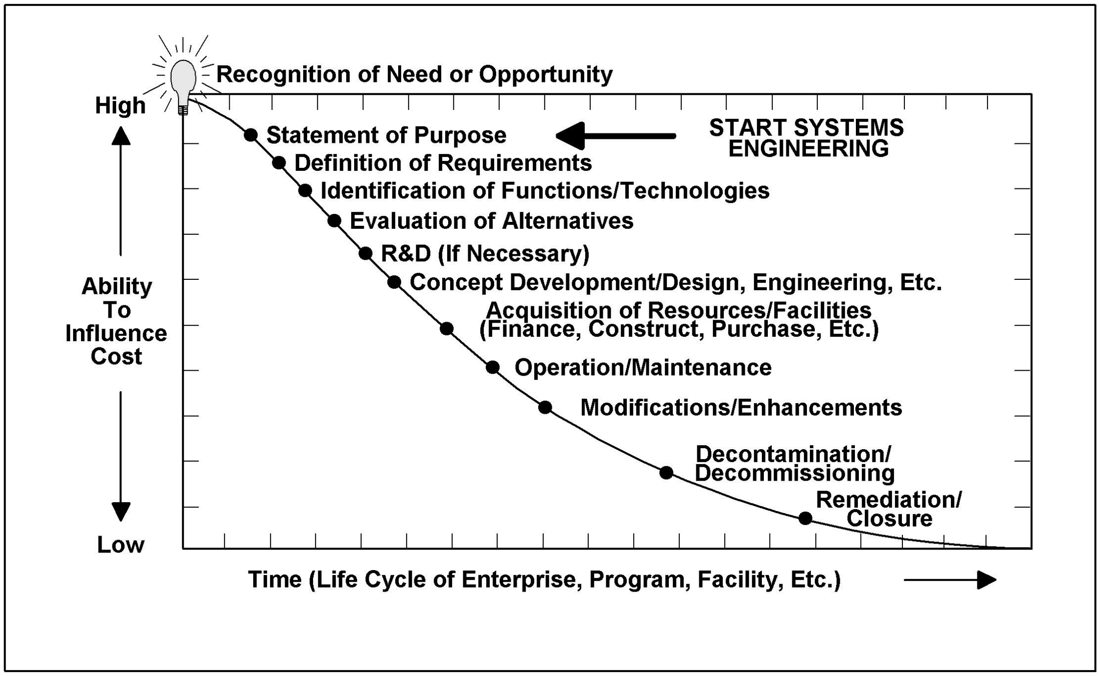

Figure H-9. The systems engineering process should be started early for maximum benefits with respect to achieving low cost.

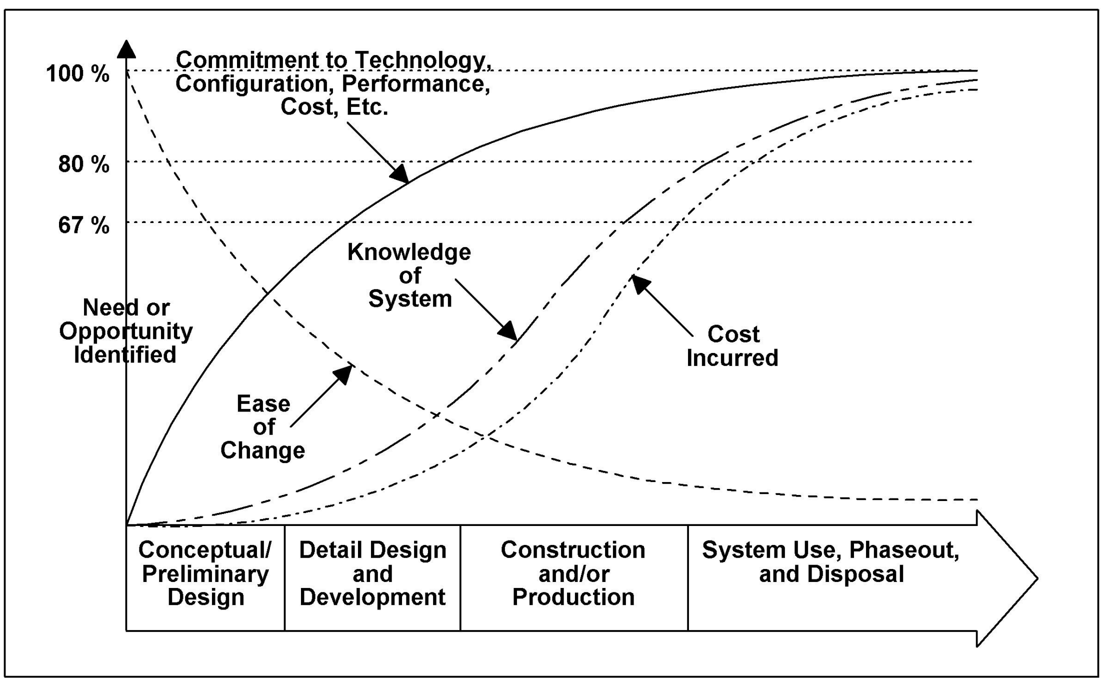

Figure H-10. Commitment to technology, configuration, performance, and expenditure often occurs early in a project while the ease of change decreases as the project proceeds. For best results, early application of systems engineering principals is generally vital.

A commonly used methodology applied to control the SE process and ensure accountability and traceability involves the use of relational database technology. This technology is used to maintain all of the information about the design project using a formal schema, such as the widely used entity-relationship-attribute (ERA) schema shown in Figure H-8. Such data includes, but is not limited to:

- The SE team personnel and their responsibilities
- The requirements that the system must satisfy and the documentation of the origins of the requirements
- All of the characteristics of all the candidate designs and documentation of how they were derived
- Documentation that specifies where, when, why, how, and under what circumstances various events and activities occurred
- The results of all tradeoff, verification, and other pertinent studies.

Note that not all of the attributes listed in Figure H-8 apply to all of the entities listed in the figure and that not all pairs of the entities are necessarily related by all or even any of the relationships shown. The use of a relational database facilitates the efficient, organized maintenance and rapid retrieval and examination of project data and the relationships among them.

Practices and Elements of Good SE

The team developed a top-level list of fundamental practices or elements of good systems engineering, which typically includes:

- ***Requirements Development.*** This entails understanding customer needs, properly stating the problem, and accurately specifying the requirements that define what the system must do.
- ***Incipient System Design.*** This consists of defining system concept models at the beginning of the effort; identifying and organizing the hierarchy of functions to be performed by the system based on the top-level performance objectives in a process known as *functional decomposition*; defining the system constraints; defining the hierarchy of physical elements (e.g., subsystems and individual components) through a process *called physical decomposition*; and allocating detailed performance and interface requirements to the physical elements.
- ***Evaluating Alternative Concepts.*** This involves identifying, developing, and establishing the relative merits and drawbacks of alternative concepts using a design tradeoff methodology. The methodology used may be formal or informal (preferably formal) and it uses the results of analyses, simulation model testing, and/or physical model testing.

- ***Make-or-Buy Decisions.*** This involves determining whether the system or one or more of its elements should be constructed in-house by the system developer or purchased from an outside source. Important factors involved in making such a decision include availability, cost, quality of commercial offerings, the requirements for the system being developed, and the protection of, or a desire to expand, core competencies.
- ***Validation.*** Validation consists of ensuring that the established requirements are consistent with customer needs and that a real-world solution can be built and tested to prove that the requirements are satisfied.
- ***Verification and Integrated Testing.*** This involves the determination of design compliance with performance specifications and the compliance of hardware and software with specifications. Validation and integrated testing includes (1) identifying individual-component-level through subsystem-level to complete-system-level testing and inspection in a test and evaluation master plan early in development, and (2) actually conducting the tests and inspections in a complete and logical manner for individual components, subsystems, and the integrated system.
- ***Configuration Management (CM).*** CM refers to establishing and maintaining the status of the design configuration and interfaces, as defined by specifications; controlling changes to the configuration; appropriately controlling changes between subsystems and the system and the external world; and maintaining the traceability of the configuration as it changes.
- ***Production Considerations.*** This is defined as addressing and giving adequate priority to the production considerations early in system development, with the objective of allowing production considerations to influence the design of the systems to reduce costs and ensure quality, where appropriate.
- ***Subsystem Integration and Technical Management.*** This element of good SE involves bringing components and subsystems together not only to produce the desired results, but also to ensure that the interactions of the system elements and the performance of the system as an integrated whole satisfy customer needs. It includes organizing the technical effort and identifying how the development will be broken down and managed; integrating the activities of the development team; balancing the influence of all required design specialties; resolving design conflicts; ensuring the compatibility of all physical, functional, and program interfaces; and assessing and managing technical risk.
- ***Life-Cycle Considerations.*** This refers to giving due priority to long-term issues with appropriate requirements and objectives. Such issues may include supportability, maintainability, reliability, training, and life-cycle costs.
- ***Program Management.*** Program management involves planning, tracking, and coordinating activities performed by all elements of the development team, as well as resolving impediments to program progress. Evidence of strong program management includes an integrated master scheduling system; an efficient cost accounting system that

provides for the management of the development process in a timely manner; life-cycle cost estimates; risk analyses; and regular program reviews with all key stakeholders.

In general, all of the above elements must be accomplished as part of effective SE, but the necessary extent and formality of the application of these good SE practices usually depends on the particulars of the system being developed. These elements and practices are intended to ensure that the traditional activities of engineering design, tradeoff-study, modeling, simulation, design of experiments for testing and evaluation, etc., are properly coordinated and performed efficiently and effectively, especially in a concurrent engineering environment. An issue for any MS&A project is to what extent and how formally the elements of good systems engineering practice are to be applied. Team members concurred that the development of the kinds of integrated, life-cycle decision support MS&A tools discussed throughout this document could benefit from the application of SE methodology.

An important part of good SE practice is ensuring that the desired level of quality is maintained throughout the process and for the products of the SE effort. A number of methods exist for achieving high quality, and these methods can be applied informally or (preferably) formally. Part of the process of ensuring quality is addressing standards. The issue for MS&A projects is determining which methods and standards to apply, and how formally. The quality assurance aspects of SE can help to ensure that MS&A tools developed using SE methodology, and the results generated using these tools, are useful to decision makers and accepted by stakeholders and the public.

Business Process Reengineering and Privatization

- ***Business Process Reengineering*** (BPR)—is defined as the radical redesign of business processes to achieve dramatic improvements in performance. BPR can be viewed as an application of SE that is currently of particular interest to DOE, DoD, EPA, and other government agencies.

- ***Privatization*****—**is generally used to mean the contracting by government with commercial firms or private sector not-for-profit organizations for goods and services that were formerly provided by the public sector. Of course, BPR of purely governmental functions without privatization to reduce costs and/or improve services and products through enhancements in efficiency and/or quality is also of on-going interest to government agencies. Because of its overall magnitude, privatization of EM-related infrastructure can be big business. It is hard to imagine a more radical redesign of business processes for government organizations than privatization of activities traditionally performed by government.

Potential benefits of privatization, which are not always realized in every case, include using the generally observed greater efficiency of the private sector relative to the public sector for many business activities; accessing the ability of the private sector to tap funding sources not available to the public sector; transferring risk to the private sector from the public sector; circumventing constraints on the scheduling of activities by government (e.g., by better matching of expenditures to budget cycles); reducing capital outlays required of government; achieving economies of scale; and satisfying voter demands for the downsizing of government.

There is also a price to be paid for these benefits of privatization: (1) In addition to compensation for the direct costs of goods and services, the private sector expects to profit from its involvement in a privatized activity. (2) The anticipated profit must be commensurate with the perceived risk so that, in general, higher profits will be demanded for the assumption of liability for damages and financial risks significantly higher than that typical of normal business. (3) Commercial entities generally avoid assuming risk that threatens their existence, so limits on liabilities implemented in various ways are often demanded. (4) There are various current functions of government for which the ultimate responsibility is viewed as residing with government, so that even when these functions are privatized, there is a need for continuous, vigorous oversight by government, which may require significant resources. MS&A can aid in establishing appropriate profit levels and limits on liability and providing effective oversight.

Full-scale SE, including all appropriate MS&A, should be performed for the actual systems design for complex privatized activities. This generally should be the responsibility of companies offering to perform the privatized activities, but government should insist on it being adequately done. Government also should perform in house (or cause to be performed by independent contractors for complex privatized activities) independent SE adequate to promote the formulation of good requests for proposal for privatization; the effective evaluation of responses to such proposals; the writing of good contracts; and making the administration by DOE, DOD, etc., of privatized activities more effective. SE may also prove useful in the commercialization of complex emerging technologies developed at the behest of DOE, DoD, etc.

Questions and Answers

The interest area team addressed the twelve questions given to the teams as guidance, attempting to provide at least a general answer to each of the questions while acknowledging that with respect to some, the depth and breadth of relevant experience of its members were limited. In addition, because of the very broad scope of the natural and artificial systems, processes, and activities that fall under the definition of infrastructure at one or more federal agency organizations, or those of their contractors, and because of the time constraints of the workshop, an in-depth treatment of every infrastructure category and topic for every scope, scale, and time frame with respect to each of the questions was not feasible. Consideration of the detailed questions was guided by the more general charge to the workshop participants to produce recommendations for the further development and application of MS&A models, techniques, and tools where appropriate. In various instances, the team took the liberty of rephrasing the questions that were originally posed.

1. What are the important problems to be addressed by MS&A, including broad issues such as political, economic, safety, societal, etc., concerns, for the interest area?

The team discussed the detailed lists of infrastructure general categories, scopes, scales, and time frames, and specific topics listed in Tables H-1 through H-3. The modest size of the team, and hence the limited breadth of the experience of its members, plus the available time, did not permit a definitive prioritization of all of the problems in all of the infrastructure categories listed in Table H-1 with respect to all of the scopes, scales, and time frames and topics listed in Tables H-2 and H-3. However, the following general categories were identified as being particularly important:

- The processing of radioactive, chemical, and biological wastes to render them innocuous or to convert them to forms suitable for interim storage or ultimate disposal, and the cleanup of sites contaminated with such wastes.
- Transportation in general because of the emissions (including toxic wastes, such as sulfur and nitrogen oxides and particulates), and greenhouse gases (e.g., carbon dioxide from roadway vehicles, railroad engines, watercraft, and aircraft fueled by fossil energy), and leaks of fuels during delivery and use. Transportation in particular because of radioactive, chemical, and biological wastes, including packaging and handling.
- The interim storage and final disposition of radioactive, chemical, and biological wastes.
- Electric power production fired by fossil fuels because of emissions from generating units, including toxic wastes and greenhouse gases.

The criteria used in assessing importance included complexity with respect to the decisions to be made and the total economic, human health and safety, and other societal and environmental impacts.

2. Which questions in the interest area can be answered through the application of MS&A methodologies and tools?

The list of topics presented in Table H-3 illustrate in skeleton form the breadth of “what, where, and when and which, what kind of, and how many” questions that can be answered by the application of MS&A methodologies and tools.

3. What are the magnitude and the imminence of each important problem identified for the interest area?

In general, team members agreed that when any of the problems identified by the team as being particularly important for each of the general categories of infrastructure are not adequately addressed, adverse consequences may result. For problems that are identified as being of greatest significance, there can be large and long-lasting economic, human health and safety, environmental (ES&H), political, and other environmental and societal consequences. Although some of these problems have been partially solved, the current environmental and societal impacts resulting from the incompleteness or nonexistence of solutions for all the problems were judged to be substantial by the team.

4. What is the current level of MS&A effort directed toward solving each of these problems relative to their perceived importance?

The team noted that substantial resources were currently being devoted to the solution of most of the problems identified as being of greatest significance for the infrastructure categories that were judged to be of highest priority with respect to MS&A to support EM. Such investments in MS&A are being made by U.S. government agencies, including the agencies sponsoring this workshop, and others represented unofficially by individuals participating in the workshop, academia, state and local governments, foreign governments, and international organizations. The team perceived some MS&A efforts with respect to some problems as being in their infancy. These efforts include global climate changes of anthropogenic origin, which are expected to be driven largely by carbon dioxide emissions from fossil-fueled electric power generating stations and motor vehicles and other transportation sources of emissions. In the case of climate changes that may be driven by carbon dioxide, the absolute significance of the environmental and societal problems that may result from the changes are difficult to establish definitively. The primary reason for this is because of limited understanding of the phenomena involved and the available data. However, such problems may turn out to be among the most important of all those facing humanity. Further MS&A can help to definitively determine the significance of these problems. Decision makers are just beginning to appreciate the magnitude of the MS&A effort needed to complete this phase of addressing the issues of potential climate changes due to human activities. The magnitude is perceived to be substantial because of (1) the size of the problem with respect to both geographical extent and potential societal, economic, and political impacts; (2) the complexity of the problem, with the involvement of the entire biosphere and lithosphere (in addition to all of man's activities, institutions, and works) among the natural and artificial systems that can be significantly affected; and (3) the inaccessibility to any, or at least to timely, experimental investigation of many of the phenomena that are expected to play significant roles in climate changes.

Large increases in the magnitude of the MS&A resources devoted to preventing or mitigating undesirable impacts of climate change, where deemed cost effective, will be justified if it is determined that the societal and environmental impacts resulting from changes in global climate caused by man's activities will be unacceptable or if ways to prevent or adequately mitigate the consequences of the changes are not developed.

The adequacy of the MS&A resources devoted to recent government efforts at site remediation, waste treatment, and disposal, and the privatization of such activities and examination of the consequences of decision making that affects EM activities, appears questionable. On the other hand, MS&A for many EM-infrastructure-related design, construction, operations and maintenance, systems and activities are often adequate when performed by the private sector in the ordinary commercial environment. This is because the investment in MS&A needed for cost-effectiveness has been more or less accurately established.

5. How can it be determined when enough MS&A has been performed for a particular issue, question, problem, project, program, etc.? Have MS&A models, techniques, and tools been used in this interest area, and, if so, which ones?

It must always be recognized that any investment in MS&A involves the expenditure of various resources and that a satisfactory return on the investment will not always be forthcoming. At one level, enough MS&A to aid in solving a problem has been performed when a satisfactory (at least for the moment) solution to the problem has been developed. If there is a perception that a superior solution exists with satisfactorily high probability, continued MS&A to address the problem may be justified. This is the case provided that (1) the added value of the new solution exceeds the cost of implementing it and (2) where necessary, the added value exceeds the cost of eliminating the previous solution plus the cost of the additional MS&A and other activities to develop the new solution. MS&A to support the making of a decision that cannot produce the necessary information in time to impact the decision is clearly of little use with respect to the making of that decision.

On another level, in some instances it is theoretically feasible to estimate the marginal return on added investment in MS&A for a particular project. It is also feasible to estimate the economic consequences of deciding a particular question in various ways and to compare the results with estimates for the MS&A necessary to reduce the risk of undesirable outcomes and the amount by which the risk could be reduced. In many cases, the appropriate amount of EM-infrastructure-related MS&A has been relatively accurately established by experience. Decision makers should keep in mind the difference between MS&A for RDDT&E (for which the uncertainties involved and hence the risk of not obtaining useful results can be large) and MS&A to reduce risk in conventional design and other decision-making activities (where the appropriate amount of MS&A and the kind, quality, and value of information to be produced is often known with reasonable certainty).

At still another level, the question to be addressed is the perception of decision makers concerning the value of the information to be obtained through additional MS&A relative to the cost of producing it. The value is determined by the impact of the information on the consequences of decisions based on the data relative to those decisions made without the information, perhaps quantified in strictly monetary terms, but also often reflecting the value system of the decision makers. There is also the cost of whether the desired information can be produced in a timely way with respect to the decisions to be made. When the value of this information is perceived to be significantly greater than the cost of producing it through MS&A, and the cost of obtaining it in this way is perceived to be significantly less than the cost of acquiring it in other ways, the decision is likely to be in favor of additional MS&A. Otherwise, the question of additional or no more MS&A is likely to be decided differently. If the perceptions of decision makers with respect to the value and/or the cost of obtaining the desired information—either through MS&A or in some other way—are seriously flawed, the MS&A community must attempt to correct these misconceptions.

Various widely used and accepted MS&A models, techniques, and tools are used to address problems in this interest area. These models are continually evolving, and some are relatively new.

The models, techniques, and tools that have been applied in the infrastructure area include ones that have been invented and developed under the aegis of various federal agencies, in academia, and by private companies. They include public domain and commercial software packages for building models, performing simulations, and analyzing results.

The subject categories of these models, techniques, and tools that are generally considered to relatively well-established in the infrastructure arena include:

- Systems engineering
- General-purpose continuous and discrete simulation, and combined continuous and discrete simulation, of various kinds of transient systems. These include complex systems with natural and artificial elements, such as environmental, contaminated-site remediation, waste treatment, packaging, transportation, storage, and disposal systems, as well as business, economic, political, government, and other social systems
- The design, operation, and control of steady-state chemical process trains, flow systems, and networks of various kinds
- Cost estimation and modeling
- Risk analysis
- Decision support
- Specialized continuous and discrete simulation, and combined continuous and discrete simulation, of business processes, business process reengineering, manufacturing, and work flow.

One of the newer kinds of MS&A for EM-related infrastructure is *object-oriented microsimulation* of transportation systems, in which the characteristics and behavior of large numbers of more or less similar elements of a complex system are specified and simulated individually. An example of such a system might be one composed of a highway network, drivers, traffic control elements, and vehicles, which includes many identical elements that are: (1) constrained differently; (2) operate with different characteristic spatial and temporal scales and resolutions; and (3) require the inclusion of different levels of detail to achieve satisfactory results.

6. What can be done with MS&A in this interest area, with examples of success and non-success where known?

The team felt that, to a greater or lesser extent, and at one time or another, MS&A has been applied for EM RDDT&E and the design of EM infrastructures for virtually all of the infrastructure categories, scopes, scale, and time frames, and topics listed in Tables H-1 through H-3. Such MS&A may have been part of a systems engineering process and/or used to support EM decision making. Many excellent results have been obtained. Unsatisfactory outcomes of MS&A activities typically appear to be consequences of model inadequacies, insufficient resources, or inadequate data. Model inadequacies are often due to insufficient understanding by the modelers of the problems to be addressed and the phenomena to be modeled. Another cause is approximations, simplifications, or model incompleteness that results in significant behavior, including emergent behavior, that is not detected. When resources are insufficient, all the important factors and issues may not be fully examined.

There have been numerous instances where government agencies have funded the development of potentially highly useful MS&A software and databases, but have failed to follow up adequately. In some cases, potentially valuable products were funded for development only up through the demonstration phase and then allowed to languish. Further funding and development might have made these products truly useful, or made them available to commercial development firms. Even when products are developed to the point at which they became useful, adequate funding for continued maintenance and upgrading often is not made available, so the products are replaced by other government-sponsored or commercial products. In many cases, the net effect has been that potentially valuable products have effectively disappeared. This commonly occurs when the products are not well documented; the documentation and the products themselves are not securely archived in a way that permits ready determination of their existence, assessment of their potential value, and retrieval of the documentation and the products for use. There are several reasons for this:

- Changes in personal priorities or incumbency at the level of the decision maker that originally funded the work
- Changes in policy and/or budget priorities at higher levels
- The person or team that originally developed the product is transferred to other work, or are incapacitated (e.g., through death or retirement), and there is no replacement or effective transfer of ownership and corporate knowledge
- Customers for the product “disappear,” perhaps only temporarily.

An effective MS&A infrastructure could prevent such losses of potentially valuable MS&A products developed at public expense.

7. If MS&A are not being used in this interest area, then why not?

The team members generally agreed that MS&A has been, and is continuing to be, used on a more or less routine basis in the infrastructure interest area. However, they also agreed that more MS&A could and should be performed to support EM activities in this interest area; more effective use could be made by decision makers of the information produced by MS&A; and it is important that the MS&A community take steps to convince decision makers of the value of more MS&A and to see that decisions makers get their money’s worth.

8. Are there gaps between the development of MS&A models, methodologies, and tools and application in this interest area, and, if so, what are they?

The consensus of the team members was that existing and emerging MS&A models, techniques, and tools are adequate to address most, and perhaps all, of the infrastructure problems that have been identified. However, they are satisfactory for the moment; there is always room for improvement in such areas as ease of use, sophistication of output, more efficient algorithms, documentation, the detail treated by models, and the scope addressed by models. The real problems with respect to MS&A models seem to be a lack of interest on the part of decision makers in supporting more extensive MS&A, a lack of data adequate to justify the application of sophisticated MS&A in some instances, and the limited availability of resources to do as much MS&A as could be reasonably justified. The first problem, a lack of interest, may be fixable through better understanding on the part of the MS&A community of the requirements and desires of decision makers, greater efforts to satisfy decision makers, and better understanding on the part of decision makers of what MS&A can do for them in a timely and cost effective way;

9. Have cost/benefit studies been conducted for various MS&A models, techniques, and tools used in this area and, if so, what are the principal findings of these studies?

The team was not aware of any studies that specifically addressed and reported on absolute costs versus benefits of MS&A, even for narrow categories of models, techniques, or tools. Truly useful cost/benefit studies might have to include the following:

- The determination of all of the contributions to the total cost of MS&A. This determination would take into account (1) the costs of acquisition, maintenance, application, and utilization of results (e.g., purchase or license, training, personnel, equipment), (2) the total cost of applying MS&A throughout the useful service life of a model, technique, or tool for multiple applications or for a specific project; and (3) the costs for new development required for a specific application. Development costs for pre-existing models, techniques, and tools are not included.
- The identification of all the benefits, with a monetary value assigned rationally to each benefit for the entire period when such benefits accrued. This might include times long after the MS&A itself was completed.
- An analysis of a specific application under specified conditions, or of a scenario that included typical applications of mature models, techniques, and tools. Pathological situations are not included.

These are not trivial tasks. Because their performance requires the investment of significant resources, they are rarely undertaken. Some published results of case studies indicate more or less quantitatively the value of MS&A, but team members could not cite specifics.

Some team members were aware of numerous anecdotal reports in trade literature concerning some information about the general usefulness (and some of the cost of ownership and operation) of various kinds of commercial software and hardware. Also, there are research-oriented reports concerning various models, methodologies, and tools in the professional literature. These reports are usually prepared by proponents of such products. In addition, various surveys and assessments have been conducted and the results of comparisons of features and costs for software and hardware have been published. Some of these reports have been published in trade and professional journals; others have been sponsored by various government agencies, with the results published in technical reports.

10. What MS&A models, techniques, and tools are shared with other interest groups represented at this workshop?

Team members indicated that the application of SE principles, tools, and MS&A efforts could prove beneficial to many EM activities in all the interest areas. In the Infrastructure interest area, MS&A could be used to aid decision for:

- Project management
- Business process simulation, including privatization and workflow analysis
- Cost and economic modeling; formal decision support
- General-purpose discrete, continuous, and combined discrete and continuous simulation
- Models, techniques, and tools, plus some relatively new object-oriented microsimulation models, techniques, and tools, such as those being developed in the transportation arena.

Many of these techniques and tools are already being used to some extent in some of the other interest areas. More extensive application of them may be warranted in at least some interest areas, including the Infrastructure interest area. The MS&A traffic flows in both directions. Various MS&A models, techniques, and tools usually viewed as specific to other interest areas are used in the Infrastructure interest area. Prominent examples include tools used for chemical, radiation, and radioactivity fate and transport and process design. Results obtained by workers in the other interest areas are needed for further work in the Infrastructure area.

11. What are the perceived benefits of MS&A for the resolution of EM-related infrastructure issues?

The team discussed the perceived benefits that can be realized when MS&A is used to support decision making in the EM arena. The following are some of the conclusions that were reached.

- Benefits can be realized when projections far into the future are involved, such as when designing strategies that use natural phenomena or artificial structures for the containment of radioactive wastes in engineered repositories for more or less permanent disposal. Another example is when the transport and fate of groundwater pollutants must be predicted to address the issues involved in selecting long-duration remediation alternatives. In this case, only MS&A can generate the needed information. The distant future is not accessible through experimentation.

· MS&A is beneficial when the scales (spatial and temporal) of systems or the complexity of systems on which experiments might be conducted makes it too difficult to obtain the desired information. In this case, MS&E may be the only feasible approach. For example, it is generally not feasible to do experiments at astronomical scales, at global or continental scales on earth, and over geologic time. Only MS&A can compress spatial and temporal scales to generate useful information about such systems at acceptable cost. Infrastructure systems (e.g., economic, political, and transportation and communications systems) also fall into this category of situations in which useful experiments often are not feasible, but MS&A may be.

· MS&A is beneficial when experiments cannot be controlled very well, when the deviations are not well-known, the phenomena being investigated are poorly understood, the systems being studied are so complex that the collection and/or processing of sufficient data to adequately characterize them are not feasible, sufficiently accurate measurements cannot be made, and/or information obtained through experimentation may be misleading. It may be possible to obtain more useful information through well-understood MS&A, even when the models are highly simplified and approximate.

· MS&A is beneficial when the subjective risks of various kinds (e.g., financial, ES&H, political) or the objective risks calculated for potential unfavorable outcomes are perceived to be too great. When authorities have the power to prevent them, permission to conduct the experiments is unlikely to be forthcoming. This leaves only MS&A to provide the desired information. Unfavorable outcomes may arise naturally because of inherent characteristics of the systems involved, inadequate inability to control the course of experiments, or unanticipated phenomena, such as various kinds of emergent behavior. For example, take the case of the seeding of a hurricane with inorganic microcrystals to accelerate the release of moisture as rain from the clouds around its eye in an attempt to reduce the hurricane’s maximum winds. This was tried at least once with ambiguous results, and it is unlikely that such an experiment will be attempted again any time soon because of public perceptions about the potential consequences. Meanwhile, extensive MS&A for hurricanes has been, and is still being, performed by various researchers to provide information useful for long-range weather forecasting, the design of structures, and the formulation of evacuation plans.

· MS&A is beneficial even when the anticipated rewards from successful experiments are substantial. Unfavorable public perceptions of risks associated with undesirable outcomes may impede, or even prevent entirely, experimentation. For example, much of the public in the U.S. and abroad is wary of the potential impacts of possible unfavorable outcomes of experiments involving nuclear phenomena and genetic engineering, with well-known consequences for constraints on experimentation, even though potential rewards are great. In such cases, there is often no significant opposition to MS&A.

· MS&A is beneficial when there are phenomena, technologies, and systems whose theoretical basis is sufficiently well established and/or the base of empirical experience is adequate, existing models are well-established and widely accepted or accurate new ones can be constructed quickly at low cost, and the solution algorithms and/or simulation tools are known to be sufficiently accurate and efficient. In such cases, acceptable, or even superior, results often can be obtained more quickly and/or cost effectively through MS&A than by conducting experiments, even when the experiments are feasible. In many instances, the dominant costs for generating information through MS&A are associated with the formulation and verification of the model with which simulations or calculations are performed and/or obtaining the input data. In such instances, virtually unlimited quantities of results can be obtained at little additional cost once these steps have been completed.

· In many cases, experiments are not only feasible, they also can provide all of the data that is desired at acceptable accuracy, sufficiently quickly, and at attractively low cost, as well as establishing credibility as only empirical results often seem able to do. Even in such cases, MS&A can occasionally be applied to generate information that is useful in designing experiments to produce results of greater accuracy more quickly and cost effectively, even when the added cost of the MS&A is included.

· Even when experiments can produce all of the necessary data more accurately, quickly, and cost effectively, MS&A often can generate information, which, while perhaps of lower accuracy, usefully supplements the experimental results. For example, data generated for regions of parameter space that are not accessible by experiments can foster insights that aid in promoting improved understanding of the phenomena involved and faster, more accurate, more cost effective evaluation and interpretation of the experimental results.

· MS&A can treat nonexistent and conceptual systems in terms of shedding light on real systems of interest. These systems can be used to conduct Gedanken (thought) experiments and “prove,” using numerical methods, mathematical theorems for which no analytic proofs have yet been devised. They can also be used to generate realistic results for very wide regions of parameter space much more quickly than through experimentation and can be used in many system configurations for purely illustrative purposes or to perform tradeoff studies, answer “What if” questions, and produce results to guide thinking, inform, or teach.

The “experiment” of global warming induced by anthropogenic emissions of carbon dioxide probably will be conducted over the next few hundred years unless counteracted by mitigation technologies, societal changes, and/or phenomena of which people are presently unaware. Some projections of the consequences of performing this “experiment” are so dire that many people are unwilling to allow it to continue. This is a largely uncontrolled, potentially very costly “experiment.” It is very large scale, greatly complex, of long duration into the distant future, and involves enormous risks. Many people would prefer to replace this experiment with more MS&A.

12. What metrics can be used for assessing how well MS&A techniques and tools address the problems treated, the needs of decision makers, and how cost effective they are?

The members of the team recognized that the effectiveness of MS&A techniques and tools in generating useful information for decision makers can vary depending on the circumstances. Different kinds of information are needed for different kinds of decision making, and the packaging of the information necessary to induce decision makers to use MS&A varies from one situation to another. For example, MS&A to support final design decisions may include the generation of copious detailed data about geometries, sizes, materials, concentrations, and other characteristics, while MS&A to support the selection of one technology over another may focus on the development of integral measures of cost effectiveness; technical, financial, and ES&H risks; and acceptability to regulators, the public, and other stakeholders. Other examples of how effectiveness can differ from one scenario to another include the value of the information produced; the rapidity with which it can be produced once the need for it is recognized; time limits on decisions and postponements that might affect the results; the cost of producing the information, and the ease of evaluating and interpreting data.

One of the considerations in holding this workshop was the widely recognized problem of getting decision makers to make use of the results of MS&A as a routine part of business. How could decision makers use MS&A efficiently and cost-effectively in conducting many EM projects and programs, especially during the design phase? How could MS&A be used directly or in modified form as an aid to decision making? Thus, a relatively obvious measure of the effectiveness of MS&A techniques and tools in addressing the needs of decision makers is whether or not the decision makers consistently used the available results obtained in a timely manner when applying the techniques and tools. The best measure appears to be data collected for the application of each particular technique or tool or combination thereof for numerous trials with different modelers and decision makers. Evaluating such a metric may require the investment of significant resources. A refinement would be to ask the decision makers how satisfied they are with respect to the quality of the results, how easy it is to get the desired results in a timely way, and how they perceive the value of the information obtained relative to the cost of producing it.

Cost effectiveness for a specific MS&A technique or tool or combination thereof can be measured in various ways. For example, we could attempt to establish the value (see question 9 above) of the information provided to decision makers for typical scenarios and then compare this information with all the applicable costs of producing specified sets of information and packaging it in specific ways for decision makers.

Appendix I. Manufacturing/Pollution Prevention

Manufacturing/Pollution Prevention Interest Area Team

Butner, Scott—Chair
Marchetti, John A.—Chair
Boak, Jeremy—Reporter
Baker, Jim
Bluck, David
Cabezas, Heriberto
Cormier, John
Diwekar, Urmila
Kjeldgaard, Ed
Krahl, David
Lave, Lester
Lee, H. N. (Sam)
McPherson, Elizabeth
Persichetti, John
Sikdar, Subhas
Weinrach, Jeffrey
Wheelis, W.T. (Ted)

This interest area team focused on the application of modeling and simulation to the improvement of manufacturing and other industrial processes, especially for the purpose of reducing the toxicity and volume of releases of waste materials to the environment.

The team spent relatively little time on the questions of validation and performance measurement, and the history of the application of models. They did not discuss whether modeling results were reaching the hands of decision makers in government or industry. Pollution prevention success may result from management choices derived from personal, conceptual models of best business practice. No assessment was made of whether the adoption of pollution prevention principles and practices was being driven by the results of models running on silicon-based or carbon-based computers.

Problem Statement—There is a need for modeling and simulation to support decision making. Decision modeling is important; life-cycle analysis and decision methodology development support better informed decision making.

The interest area team examined improvements at all stages of the life cycle of production facilities—permitting, design, construction, operations, decontamination and decommissioning, and remediation of past facilities. Less emphasis was placed on the decommissioning and restoration areas because these were incorporated in part in other interest areas.

The team reviewed efforts in modeling and simulation of detailed industrial processes, such as chemical process models, as well as decision-aiding tools that may not model processes explicitly. Cost/benefit models, value of information models, and risk-based prioritization models were included. An additional area of examination was analytical tools for evaluation of parameter uncertainty and sensitivity, and for sophisticated data visualization.

Modes in Which Models are Used

In the environmentally conscious Manufacturing/Pollution Prevention area, models are used in three somewhat distinct modes. For each mode, the degrees required of technical rigor and completeness, ease of use and clarity, and testing and validation vary significantly.

1. The first mode in which models are used is the evaluation and ranking of options, which may be technological, economic, or programmatic. Models for this mode commonly require substantial rigor, and testing.

2. The second mode in which models are used is illustration and education external to the modeling community. Education is, at its best, a two way street—a fact commonly recognized, but not so commonly acted upon in the community of modelers and simulators. Models for such purposes have very stringent requirements for clarity and, ideally, for ease of use.

3. The third mode in which models are used is presentation and argumentation over results within the modeling. Here, models can be central to focusing discussions of problem definition, terminology, boundaries, assumptions, methods, solutions, conclusions, and needs for data or model development. Increasingly, modeling tools are expected to be able to serve, or at least be translated among, all three modes.

Questions and Answers

The team discussed and answered some of the workshop questions as follows:

1. What are the important problems to be addressed by modeling and simulation?

Discussion: The team defined the following characteristics for an optimization function or model:

- It should effectively simulate dynamic situations.
- It should have a defined objective function.
- It should meet the ultimate goal of sustainability.
- It should incorporate qualitative as well as quantitative information to support decision making.
- It should have an approach to validation in an area of sparse data.
- It should be usable as a communication tool, beyond the pure demonstration of validity (for example, the representation of wastes as “negative value products”).

- It should go beyond the technological context of particular problems, to address less technical drivers of managerial decisionmaking.
- It should focus on the prevention of generation, rather than on identifying new product potential in "wastes."

The team summarized its discussion of major questions for pollution prevention modeling and simulation in a series of fundamental questions, which were ultimately considered applicable to a wide range of problem areas.

Modeling Question	Task Title for Problem Area
What is the problem area?	Problem Definition
What do we want?	Goal Definition
What do we know?	History Matching
What else do we need to know?	Uncertainty Analysis
What can happen?	Prediction
How can we choose?	Prioritization
How can we show what we know?	Visualization/Communication
How can we test what we know?	Validation
How much is enough?	Performance Measurement

Recurring themes in most of the discussions were the need to define the area of inquiry and the suggestion that focusing on a single area might make developing a coherent view easier. Was this workshop to focus solely or primarily on DOE problems? Was the focus broader, incorporating the attempt to understand not only the needs of other governmental agencies (the co-sponsors DOD and EPA, for example) and of industry? Would a consideration of a particular problem help to integrate our answers to the workshop questions?

2. Which questions in this area can be answered with models?

Discussion: Pollution prevention is not widely accepted, regulations are not effective in making it work, and culture change is needed.

Therefore, the question of whether a problem area was amenable to modeling and simulation could best be resolved by asking, "Will it change the culture?" The team discussed the value of models as a means to demonstrate effectively the value (negative or positive) of particular actions, that is, to communicate risk in order to change behavior.

A critical lack in much of DOE's technology development efforts has been some evaluation of what changes culture, especially in positive ways. If pollution prevention is essentially a cultural change, where are the behavioral aspects in pollution prevention models? This point led to identifying behavioral modeling as a critical need, but also to discussion of the links from modeling and simulation to decision-making, through multi-criterion evaluation of options (tradeoffs of both goals; e.g., air versus water emissions, and options).

The questions that pollution prevention programs raise start at the identification of alternative options, and lead to questions of which risks are most important, which decision criteria are most important, and ultimately, to questions of whether reasonable projections of impact can be made, and whether certain products need to be made. Some, but not all, of these questions can be clarified by models, using available data, but large areas of uncertainty are inherent in such application of models. Indeed, in many instances, it is the exercise of model construction that identifies the critical uncertainties, and focuses the discussion of goals and objectives. The results of most investigations are only widely understood when they are put into the framework of a model.

The team discussed whether pollution prevention was unusual in the realm of modeling and simulation in the immaturity of the available data on processes and pollution prevention options, compared to fields such as subsurface hydrology. There was some suggestion that pollution prevention is a considerably broader area than other disciplines represented at the workshop. These questions were considered relevant to defining the state of modeling, and the development needs, but no resolution was reached.

Sustainable Development—In a discussion of sustainable development, the issues of problem definition and goal definition again dominated. This discussion arose from the nature of the session questions, which encouraged consideration at the highest level (e.g., political, social, economic). Thus, the team was brought face to face with the importance of conceptual models of concern to pollution prevention—the ultimate goal of environmental impact of industrial processes. It was unclear whether models and simulations could reasonably evaluate sustainability, when the very definition was unclear. Sustainable development has become a catch-all for many social justice issues, from resource allocation and use, to environmental justice, population control, reduction of poverty, crime, and teen pregnancy.

The Brundtland Commission's definition, of ensuring that resources be conserved and impacts avoided for future generations, has a static and dynamic version. It is unlikely that a static definition, with no use of nonrenewable resources, could be achieved. The static definition would only be appropriate if we understood well the needs of future generations. These needs are not well understood partly because of technological advances fueled by resource consumption. However, a dynamic definition, with non-renewable resources used to create new resources (especially intellectual capital) for a future generation, may be achievable. It is important to tie any description of sustainability back to reasonable business objectives. Currently, business is only locally interested in sustainability, mainly from the viewpoint of corporate citizenship.

In summary, the team agreed that the effort of developing reasonable modeling tools for sustainable development, incorporating cost as well as resource efficiency, was likely to inform the debate over the definition and goals for sustainable development, and ultimately offered the potential to draw the interest of industrial, regulatory, and stakeholder organizations. Without clear and quantitative outputs from such models, agreement over the goals is highly unlikely. Rather than formulating a strict definition of pollution prevention, it may be more important to define the potential future environmental legacies and avoid them by whatever means.

Problem Areas for Environmentally Conscious Manufacturing/Pollution Prevention—The team discussed a possible framework for describing the manufacturing/pollution prevention interest area as a nested suite of subjects, represented as concentric rings, and proceeding inward from Sustainable Development to Industrial Ecology to Life-Cycle Analysis and Design for Environment, to Resource Efficiency (or Resource Conservation). Further inside would be the areas of Waste Minimization, Waste Treatment, and Waste Disposal. This conceptual framework is shown in Figure I-1.

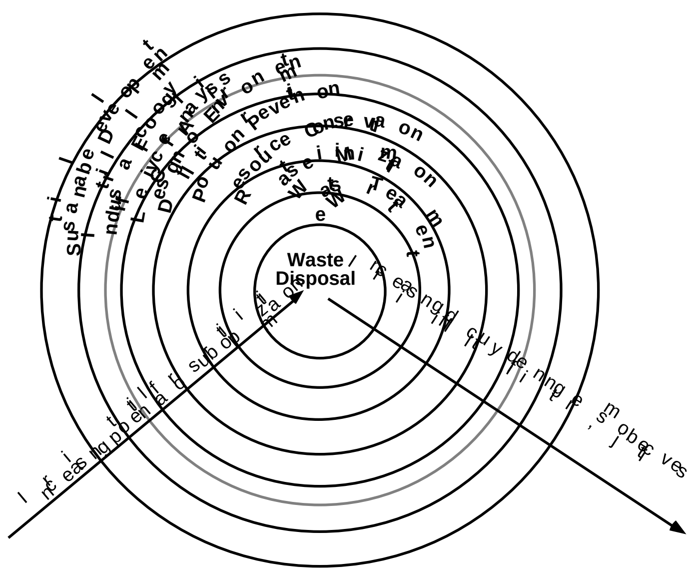

Figure I-1: Problem areas in environmentally conscious manufacturing and pollution prevention.

The outer rings generally encompass the inner rings. For example, the economic models included in the structure of Life-Cycle Analysis models are added to the mass and energy balance of process simulation tools used for pollution prevention and resource conservation. Thus, the outer rings describe more comprehensive views.

In the innermost rings, there is significant potential for unlinked systems to be locally optimal and globally suboptimal. On the other hand, as one moves toward outer rings, the complexity of the system increases, and constructing models in which assumptions, inputs, parameters, relationships, objectives, and interpretations are consistent and readily comparable to other models is increasingly difficult. The achievement of truly integrated models that simulate complex systems probably requires abstraction of more detailed underlying models. Each of the successive circles is, in the current state of modeling and simulation, represented by less advanced models, many of which are only in the development stages. Uncertainties tend to increase as one moves toward outer circles. Especially where cost becomes a consideration, the uncertainties in cost of waste avoided may well dwarf technical uncertainties.

3. What is the size/imminence of this problem?

Discussion: This model of the interest area (Figure I-1) served to focus a discussion of the question of size and imminence. Modeling at the intermediate levels may present the greatest difficulty. Lower level models that are focused primarily on physical systems are in many cases quite advanced. The highest level of models are primarily conceptual exploratory models in which significant simplifications must be made to make the problem tractable. Building bridges between these levels may be the most challenging.

4. What is the current level of effort toward solving the problem(s)?

Discussion: Questions arose about what level of consideration was needed with respect to modeling and simulation. Was it the highest level of thinking or was it looking at some very specific, perhaps DOE-focused questions? The team discussed looking primarily at routine operations, with some examination of off-normal conditions (for example, spill control) since the primary objective of pollution prevention is to prevent releases or emissions from active processes. Some consideration of all aspects was considered to be necessary.

5. Have models been used in this interest area, and if so, which ones?

Discussion: The team discussed each of the problem areas shown in Figure I-1: Resource Conservation, Pollution Prevention, Design for Environment and Life-Cycle Analysis, Industrial Ecology, and Sustainable Development. For each area, examples were given of modeling and simulation applications. The team then identified strengths and weaknesses of each class of models. The final part of the discussion attempted to assemble general needs across the classes of models, so as to define a limited set of general recommendations for the interest area.

- ***Resource Conservation (Efficiency)***

The discussion of resource efficiency modeling generally focused on areas where models had been applied successfully, generally to the incorporation of mass and energy balance. These included DOE’s American Textile (AMTEX) Partnership, which attempts to capture the entire textile manufacturing process to identify potential efficiencies. The measure of efficiency is, to some extent, market driven, leading to some resource inefficiencies, such as stressing fast but energy intensive transportation modes (air). The AMTEX program has used modeling to optimize resource utilization through inventory control, production scheduling, and material selection.

A great deal of management science is dedicated to resource efficiency without necessarily integrating the environmental view of resource efficiency in its optimization. Such areas as modeling of Just In Time processes is directed at such targets as well. Many of these exercises seek to reduce lead time as well, again, not necessarily resource conservation from the viewpoint of pollution prevention.

Chemical engineering modeling is likewise focused on optimization without necessarily accounting for environmental issues. Relatively sophisticated coal and gas turbine efficiency modeling focuses primarily on energy resource conservation, but also increasingly on emission reduction. The Clean Car initiative conducted extensive modeling of engine systems and of automobile designs to optimize fuel economy for constant performance levels. The initiative evaluated hybrid vehicles, advanced diesel engines, and others, and determined (through modeling) that only 4% of the energy used by current automobiles is used to move the vehicle; the rest is waste.

Positive Attributes of Available Tools for Resource Efficiency

— Models perform mass and energy balance well at steady state.

— Material management and tracking, as part of the balance of mass and energy, is commonly performed well by models directed at efficient resource use.

— The level of thermodynamic data in chemical process models is generally driven by demand. It is unclear whether additional capabilities are demanded by attempts to minimize releases.

— Many currently available models are easy to use, and have therefore acquired relatively broad acceptance.

Areas Requiring Refinement

— Most process models are not configured for environmental impact analysis. For example, the modification required to model well the overall mass balance, but at the same time handle the differences of large numbers required to track emissions at the part per trillion level, are not there, although they could be (there are no significant barriers except programming effort).

— Reaction kinetic models are commonly more simplified; batch reactor prediction may be less effective.

— Dynamic processing is relatively underdeveloped. Linking models to in-process data so as to replace linear programming tools for controlling processes has not been implemented.

— A variety of non-equilibrium and rate-limited processes are not commonly modeled; kinetic effects are not advanced except in limited applications. The thermodynamics of dilute solutions, necessary to understand many environmental releases, are not commonly incorporated into models directed at chemical processes.

- ***Pollution Prevention***

SEMATECH has modeled its microprocessor chip manufacturing processes (1) to reduce solvent usage and to improve reactor designs for wafer manufacturing, and (2) to test processes for ultrapure water recycle. These would appear to be more comprehensive models directed at process design, waste minimization (70% of all materials used end up as waste), and cycle time reduction, at least compared to the Resource Conservation type of model.

The DOE Clean Coal Program has used models for NO_x emissions, using an integrated approach, modeling separation processes, turbine design and gasifier designs for reduction of waste quantities.

The Waste Reduction Algorithm (WAR) is an EPA-supported tool intended to improve existing or proposed process flow sheets to reduce the environmental impact of the process. It is a conceptual approach that is not industry specific, defining a proposed multi-attribute objective function based on environmental impact.

EPA also has software nearing completion for molecular-level solvent design that evaluates potential solvents for their environmental impact (toxicity, etc.). The EPA model focuses on the prediction of performance of existing molecules, whereas a similar model under development at the Danish Technical University is attempting to provide the option of designing new molecules.

A document from a previous modeling workshop held in 1991 may provide additional examples for applications to chemical facilities. EM-50 is also thought to have produced a description of the state of modeling. The group concluded that a small set of pollution prevention models is being applied relatively widely. The pollution prevention area is not primarily defined by its models, as, perhaps, the hydrologic flow and transport area tends to be.

Positive Attributes of Available Tools for Pollution Prevention—Pollution prevention models generally capture mass and energy balance for major constituents. They evaluate alternatives qualitatively, and in some cases at least semi-quantitatively. For material substitution, for example, identification and evaluation of alternatives is reasonably well done. For some other applications, evaluation is more qualitative. The degree of effectiveness varies from application to application.

The models are considered to have been effective in raising awareness. (No examples were given. An example of a multi-attribute utility analysis of Army pollution prevention projects did not get used. This problem raised the question of whether technical success or commercial/cultural success is the appropriate measure of effectiveness.)

Areas Requiring Refinement—Many pollution prevention models do not evaluate alternatives effectively. They need better quantitative evaluation options for different alternatives. These problems result from a number of underlying deficiencies. Many pollution prevention models do not adequately model trace chemical products, and hence are limited in their effectiveness for evaluating environmental effects. Pollution prevention models do not address cost issues very effectively, if at all. Nor do they focus on issues of relevance to regulators, such as uncertainty in inputs, outputs, and conceptual model structure. Also, they are not especially effective in incorporating qualitative information. Finally, there is a perceived lack of extensibility—models are too specific to a given application; hence, the ability to define alternatives broadly is limited.

- ***Design for Environment and Life-Cycle Analysis***

Design for Environment is considered an application of Life-Cycle Analysis with a fairly specific focus. Because of this specificity, and therefore its more complete implementation at present, Figure I-1 shows this as a partially separated category of Life-Cycle Analysis. A number of models exist for various other types of life-cycle analysis:

— EPA has supported the development of the SETAC (Society for Environmental Toxicology and Chemistry) model for life-cycle analysis for hazardous chemical processes.

— EIO (Environment Input/Output Analysis) incorporates macroeconomic models and reported environmental discharge data.

— ECOSYS, a prioritization model, and decision tool developed by Ted Wheelis, uses an analytical hierarchy process to evaluate tradeoffs.

— The Exergy approach is a recently defined conceptual approach not yet incorporated into a working model. Exergy is the term applied to the irreversible energy lost in reaching an equilibrium state in a given environment. Presumably, minimizing environmental releases reduces that irreversible energy loss.

— ECOIT is a Dutch product, similar to many other pollution prevention models derived from SETAC, in that it consists primarily of inventories of materials and databases of options, not necessarily models in the traditional sense.

— DORT (Design Option Ranking Tool) is a Design for Environment modeling tool being developed by CENCITT. The two main points this system will be based on are:

  (1) Process design is as important as process operation and there are more opportunities at the design stage for pollution prevention.

  (2) Just putting the tools in designers/operators hands will not do much good if the tools are not easy to use and do not fit into what the designer/operator is already doing. If we are adding workload, it will not get done; if we are making it part of what they are already doing by giving them tools that fit into their environment (computing and cultural), they will do pollution prevention whether they know it or not (or whether they wish to or not).

— Pacific Northwest National Laboratory has developed a database of pollution prevention options in the design area with the purpose of supporting Design for Environment (P2EDGE). This could be considered a decision support modeling tool, although its classification as a model is unclear.

— Boothroyd-Dewhurst has a material selection system for manufacturing.

— A variety of universities (e.g., Carnegie Mellon, Stanford, Berkeley, University of Wisconsin at Madison) are engaged in model development in the area of design for disassembly, which involves very detailed process simulation in manufacturing, and encounters serious combinatorial problems. The number of options is practically infinite for a given design problem. Models of this sort are not yet linked to well-developed models for the recycled value of disassembled components.

Models for life-cycle analysis must commonly address three aspects: inventory of a potential environmental agent, effects of release of that agent, and analysis of potential improvements. Most current models address the first and last aspects, and handle the second in a very cursory manner. In addition, alternatives analysis commonly is not prescriptive; it does not necessarily include the capability to identify and recommend options. Thus, models that consist primarily of databases should be considered here because a critical lack in many areas of pollution prevention is the lack of prescriptive solutions from models. Ultimately, similar databases are likely to provide part of integrated modeling/simulation systems aimed at decision support for environmental managers. Given the objective of pollution prevention to become part of the conceptual framework of industrial/governmental operations, every manager is an environmental manager.

Positive Attributes of Available Tools for Design for Environment—Multi-criterion decision making is incorporated at least in the form of subjective ranking. Models also address a larger scale of consideration than common simulation products for industrial processes.

Areas Requiring Refinement—Quantitative decision support in the form of multi-attribute analysis and optimization is currently lacking, as are the related analysis of uncertainty and sensitivity for inputs and outputs. As mentioned above, prescriptive evaluation—providing recommended options as output, rather than simply measuring the dimension of the problem—is not well implemented in any existing model.

Positive Attributes of Available Tools for Life-Cycle Analysis—Life-cycle analysis models provide valuable insight into individual processes, in part because of their capability to provide insight into larger systems. They also provide improved intercomparisons of relatively similar options over simple pollution prevention models. They are able to provide reasonable comparison of the products of alternative processes.

Areas Requiring Refinement—The models have difficulty providing valid comparisons of dissimilar options. In addition, it is not clear that any life-cycle analysis model has adequately demonstrated full life-cycle closure. Boundaries are difficult to draw conclusively. Indeed, the existence of industrial ecology and sustainable development as conceptual frameworks points up the difficulty of bounding the life-cycle of a given industrial process.

These models are also presently slow and costly. They are therefore of limited applicability to decisionmakers, who commonly require rapid solutions from limited overhead resources. As a consequence, the return on investment of developing and applying a life-cycle analysis may be low, or at least highly uncertain.

The objectivity of life-cycle analysis models is ambiguous at best, as projections of life-cycle cost are dependent on economic assumptions, and on physical process uncertainties as well. Data quality is a major issue for life-cycle analysis, calling as it does for a predictive basis when records have not necessarily have been a high priority. Approximately 90-95% of the effort required goes to data gathering. The lack of data quality at this level commonly results in less accurate mass balance, and greater imprecision in the resulting assessment. In addition, it appears that current modeling efforts have had only very vague links to environmental impact. As an example, a study of potential modifications to a military paint booth found that material flow could reasonably be estimated, but that flocculants were imprecisely measured, water flow was not measured, and it was not clear what the proper allocation should be for half a dozen different products.

- ***Industrial Ecology***

Existing models of industrial ecology consists primarily of examples such as Kalundborg, Denmark, and Port Charles, Virginia. These are locations in which local industrial complexes have been linked so as to convert byproducts of processes from potential wastes to actual resources. These existing models indicate the necessity of incorporating behavioral and sociologic input into descriptive models. Industrial ecology models are considered distinct from models further down in the hierarchy by their incorporation of technologic and economic aspects, including the effects and values of natural system elements. They are not generally considered to include political or sociologic model elements.

A National Public Radio report on the Kalundborg example included a telling comment by one of the industrial leaders responsible for the success of this effort. He pointed out that the success of this interlinking of industry depended critically on most of the decision makers knowing each other because they lived in a small village, rather than being distributed across a large urban area. It also could only have occurred, he said, because it improved profits. It may be noted that, were it not for the environmentally laudable results achieved, these two factors would have been condemned as collusion and greed.

Models that could be used to simulate more diverse cases are sparse. It was considered possible that AT&T might have an industrial ecology model. The MASS/PINCH integration model, applied for GE by Auburn University, was considered to be one possible ecological model.

Positive Attributes of Available Tools for Industrial Ecology—The major value of existing models for industrial ecology is that they attempt to incorporate concept of closing industrial loops—accounting for environmental releases so as to identify opportunities to stop those releases through alternative use.

The models are valuable for communication, visualization, and education. Industrial ecology offers a reasonably well-developed paradigm, including working theories, external analogies, and perhaps even some descriptive mathematical rules with applicability.

Areas Requiring Refinement—Environmental engineers who have recognized the value of the ecosystem paradigm (perhaps from the systems engineering perspective) have pursued the concept without engaging ecologists, who are therefore dismissive of the existing models. Thus, the ecological paradigm may be powerful, but it has not yet been adequately applied.

Industrial ecology models are predominantly exploratory and conceptual, and therefore are limited by large uncertainties, especially in modeling long-term environmental inputs and effects. Boundaries are likewise poorly defined. As a consequence, there is little that they can provide in the way of prescriptive solutions.

Industrial ecology does not incorporate two crucial elements that are part of the biological field of ecology. First, there is no attempt to incorporate the social/behavioral aspects of interacting industrial elements. Second, there is no attempt to account for long-term evolution of the ecosystem, including extinction and drastic ecosystem change. If industrial ecology had these elements, there would be no difference between industrial ecology and sustainable development.

- ***Sustainable Development***

Models in the area of Sustainable Development fall into two types: economic models and physical models. Economic models include SOLOW. Robert Ayres at MIT has developed a different model for sustainable development. On the other hand, the Wruppertal Institute has developed a sustainability model based largely on minimizing the total mass moved of constituents of environmental concern. This concept was criticized because it lacks any recognition of the different impact of equal masses of materials (for example, radioactive materials).

Models in this area are recognized as exploratory, and their failings help focus the definition and refinement of models. Thus, the lack of consensus on approaches and goals, although it results in a lack of any means of validation of models, presents a very creative opportunity for models to literally define the field. In spite of this lack of reality, workshops are underway to define sustainability. There is a sense of urgency to the need for more realistic models so that decisions are not made that commit the government and the country to unachievable goals. It is to be hoped that such models will be used extensively in moving ahead to do this, before political models, supported by minimal data and running only on carbon-based computers, lock sustainability into unattainable objectives.

Positive Attributes of Available Tools for Sustainable Development—Current models provide a testable conceptual framework for discussion and debate; they are valuable exploratory tools. They also provide some link between the economic system and the physical environment of industry and nature. Further, they are focused on the long term, which distinguishes them from models in the inner circles of the modeling/simulation arena. This long-term focus requires attention to the socioeconomic models absent in all other modeling areas.

Areas Requiring Refinement—Most models incorporate insufficient reality, and hence are not ready to provide specific recommendations that support decision making.

The question was raised as to whether it really matters whether these models are developed, given that a great deal of pragmatic pollution prevention will proceed without modeling. Problems such as the existing environmental legacies are amenable in only limited ways to pollution prevention. Nevertheless, the interest area team felt that, in order not to create a future legacy, the attempt to model comprehensively the environmental impact of our activities was valuable.

Summary of Conclusions and Recommendations

In a wrap-up session, a question was asked of the presenter about the use of “Value-of-Information” models. The presenter responded that models to assign a risk-weighted value to various potential outcomes of characterization and testing activities have rarely been applied to DOE environmental management problems. He cited one example, an exercise to design appropriate tests to define remediation options for radionuclide migration from a part of the Nevada Test Site. Working with a team of subject matter experts to define potential studies and their various outcomes, the decision support team concluded that none of the studies proposed would be likely to change the remedial option chosen, and hence the information did not have sufficient value to warrant the cost of conducting the study. Central to the agreement of the subject matter experts was their judgment that other parts of the Nevada Test Site needed investigation for similar issues, and that characterization there would be more likely to be able to demonstrate value for decision makers.

An additional example of a value of information study is the Systems Prioritization Method (SPM) exercise conducted by Sandia National Laboratories to define a suite of testing activities to be completed prior to submittal of the compliance certification application for the Waste Isolation Pilot Plant (WIPP). This exercise ranked activity sets according to cost, duration, and probability of demonstrating compliance. DOE funded activities are based on an optimal activity set. The “Value-of-Information Model” offers a structured approach to assigning priority to proposed investigations. Although such exercises are commonly rushed, and therefore imperfect, they are superior to usual budget allocation processes for such activities (various “smoke-filled room” approaches).

Appendix J. Subsurface Contamination Working Group 1

Subsurface Contamination I Interest Area Team

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The interest area team reviewed the goals of the workshop and then answered the questions provided as guidance for workshop discussions.

Questions and Answers

1. What are the important problems to be addressed by modeling and simulation? Political? Societal? Economic? Environmental?

Discussion: The answer to this question depends on which topics the question concerns. The question of how to allocate limited resources in the most effective way depends on the problem under consideration. For example, on the WIPP project, the regulators were concerned with the amount of contaminant crossing a total boundary over a 10,000 year period. The question avoided the matter of dose. If the question had been dose-related, the problem would have been modeled differently.

In the interest area of subsurface contamination, the question boils down to safe water supply. Processes and problem size determine what goes into the model; e.g., is the entire DOE complex being considered or is this a simple problem of pressure driven flow? There is no general model. We need to be more specific about the goals and the objectives.

Conceptual models need to be developed and then numerically implemented. Reports to the public should include the development of the conceptual model and the numerical model. The public often does not understand the modeling effort, and it becomes a credibility issue. Documentation should be effective for the public. Modelers need to communicate the underlying assumptions inherent to the models. Scientific research models do not need to be explained to the public. Policy models should be transparent to the public. The history of assumptions is lost as time goes by.

DOE is not using modeling for decision making. We should start with the decision makers to determine what models are needed. Floundering around with the technical models first does not effectively translate upward to the regulators. How can a decision maker be convinced to use a model? How can we understand the decision makers' questions? Even technical models must underlie some policy decision. There actually needs to be a two-way process, where the technical models feed upward and the policy models reach downward.

Regulatory standards are developed using previous modeling studies. Regulations are based on old science. There is a lag between standards and new science. A more rapid exchange of regulations is needed, and the forefront of science should be streamlined.

The purpose of modeling is to synthesize our state of knowledge, to use modeling as a tool for predictions. There are limitations. For example, we cannot make predictions about contamination levels at wells. Instead of focusing on understanding decision makers' problems, modelers have approached modeling from the bottom up.

In the oil and airline industries, modeling efforts produce profits. In order to understand the cost saving potential of using models, DOE should use models to predict the results of baseline remediation technology and then compare the outcome to innovative technologies to figure out the cost savings involved.

There are some issues that only models can answer. We should emphasize the use of models as a prognostic tool. For example, at some sites in Russia where migration is multi-faceted and comprised of several sites and sources, modeling is the only tool that can be used to understand the site. Modeling can give the total picture of plume development, and can be used to segregate areas with little data. Only when we find out what weak areas are, can we improve a monitoring program. We also need research to confirm that models are reflective of the actual data. This is a specific problem that reflects the response of how a solution is reflective of the initial data. Another approach is validating the model, using calculations that involve research in a time-period that contains all existing data (history matching).

It is not clear why US decision makers are not interested in using models. They rely heavily on models to construct or build things. For example, the Tomsk site, a 400-m deep porous fractured media, was injected with radioactive waste following a 7-year study of the area. Well data was used to develop the model for this because sophisticated models were lacking. Analog models from oil industry were used. Oil researchers helped prove to managers that the site was OK for underground radioactive waste. The Russians have spent 30 years improving the model based on field data and are currently modeling the site's effect on the nearby river and watershed system. This has helped to prove to management that the site could still be used. The waste has not migrated outside of the site. Now the focus is on trying to extend the lifetime of the site, and a model is being developed for the region beyond the site. *We need to state very clearly that modeling is a powerful tool. None of the presentations have stated the importance of modeling. Modeling can be expensive, but it helps save money and provides a safe environment.* Disposal sites are being developed with wells; each well provides large amounts of data and the parameters that are needed. All sites are in populated areas. The models are open to the public, and the public studies and discusses the models. A NATO meeting concerned with ecological safety also analyzed the data from the models.

The team felt that the presentations did not stress that models have been used satisfactorily, yet consultants are using modeling successfully. Modeling may have been given a bad name because for years modeling studies have not been believed. Since cleanup costs have risen, modeling has become a desirable approach. However, if we are not careful, the misuse of models can continue to cause people to doubt the benefits of modeling. We need to balance model credibility with usefulness.

EM has used models to prioritize for performance assessment at WIPP, including sensitivity analysis to prioritize which studies would be performed. The result was a savings of millions of dollars and completion ahead of schedule. For the Savannah River Site, models were used to help evaluate different technologies.

Decision makers want to know the uncertainty involved. The team thought that uncertainty was a major issue. Models should be used to determine which data to collect and which resources to allocate to what questions. Probabilistic approaches can and should be used. Uncertainty in input translates to uncertainty in consequences. The public may have a conceptual model of a deterministic result, but this is not true in a geologic setting. In such a setting, the best estimate is given with error bars. The best guess does not usually agree with the actual results. Environmental issues must have uncertainties.

The question of what important issues are to be addressed by modeling should be simpler. Where is the contamination? Where is it going? Is it bad? Do we care? What kinds of models are there and how do they fit into the big picture of decision making? Are models good enough to answer the regulatory questions? Can they address things that were not done well before, things that were done well, and future siting? In general, models have been used more for long-term problems than for short-term or past problems. Perhaps you cannot use a model for prediction of actual concentrations at a particular place; however, you could possibly say where a contaminant source came from or compare remediation strategies. At present, for some questions, modeling may not be the answer.

Modeling comes in different qualities. We cannot create a model of better quality than the data that it uses. Many predictions have failed because of the data, and the model was implicated. Problems of different scale may use the same model, which may be incorrect. Uncertainty is apparent in the data and must be used to understand the nature of the model. For example, in a geologic setting, a deterministic/chaotic model may be used to better describe the geology.

Plume size, location, contaminant, and plume speed should be considered first before using an extensive modeling effort. The objective needs to be stated. For example, are we talking about a specific site, a specific period of time, and a specific series of questions? Risk allocation decisions need to be made for specific DOE sites. For example, what are the drivers, and how is the plume defined? Because it costs a lot to define plume size and speed, we should look at how relevant that is to the question. It is hard to try to design an uncertainty analysis that encompasses all uncertainties. A model should not just stop at subsurface contaminant transport; other requirements that need to be considered are the biosphere, interrelationships of source terms, etc.

The model should be allowed to determine what data to collect. Modeling results may be so uncertain that the end result is that more data are needed. Should we include a conceptual model, mathematical model, numerical model, and calibration with data? The problem is that modeling is sometimes a one-time shot. Sensitivity and uncertainty are not always addressed to determine the most sensitive parameters. The magnitude of the problem (or the consequences) may determine the amount of uncertainty analysis required. Sensitivity analysis can narrow down the number of parameters that really affect the result. Modeling expenditures do not compare with expenditures on other factors.

An example of DOE insight into what we are trying to work to is a tank farm at Hanford, where closure criteria is being developed. Everything is intertwined. Source term, losses during retrieval, what is left, inventories of different tank farms—all these things are tied together. The systems approach ties everything together, but we need to be more confident about the flux, 80-m thick vadose zone piece because we are relying heavily on that. Uncertainty analysis is being used to develop distributions of parameters. Simple models are backed up by more sophisticated models that provide the parameters. An attempt is being made to use screening analysis to understand high risk drivers, with additional characterization parameters. The process is vulnerable because consistent management backing is needed. The suite of tools can be used to answer questions, and then used again to determine uncertainty. Struggling with this screening assessment or some variation can enable a more site-wide characterization program. The intent is to apply it to more than one site. A mechanism is needed to help refine the required characterization activities.

Modeling and simulation breaks into two parts: (1) Management and decision making (resource allocation, compliance demonstration), and (2) process models (conceptual, math, numerical, subsurface to biosphere, hazards reduction). If there is huge cost associated with meeting compliance, that cost needs to be part of the assessment.

When returning to the simple questions (including time and spatial scale), how sure are we? Is EPA’s major question soil concentration? What is the performance measure? (The way results are reported is important in terms of public response.) Modeling melds the different data into a single picture of the problem. All models have built in scientific and cultural biases. For example, the European communities have different concentration drivers and time frames for their nuclear waste than the U.S. Looking at actinides in the accessible environment, the Kd in borehole is high; therefore there will be no spread up the borehole. This would be a criticality issue. A scientific bias screened out something that was potentially very important. Each model includes the biases of the person doing the modeling. Other issues are validity, stakeholder's values, and uncertainty. Uncertainty is very hard to explain to the public. When do we stop remediating or stop modeling? The suggestion was made that modeling (or data collection) can be stopped when the modeling results lie far below the regulatory limits. If results are close to the limits with overlap when uncertainty is considered, more study is warranted.

All models have uncertainty. Whether the stakeholder can tolerate this uncertainty depends on the consequences. The use and acceptance of modeling depends on the consequences. Increasingly, the use of modeling to demonstrate compliance is receiving acceptability. This shift is being made because of economics. Should cost benefit analysis be included?

2. Which questions in this area can be answered with models?

Discussion: Where is the plume going? Can we actually predict where a contaminant came from and where it will end up? The answer depends on the scale and the certainty to which we need the answer. Our mission is to outline the strengths of modeling and the weaknesses, to state the obstacles, and to develop some guidelines for regulators to use in modeling. Are there alternatives to using models against other tools for decision making? One alternative is to do the cleanup without a model. Models include intuitive models. The qualitative aspect of modeling is unavoidable. When do we cross the barrier between using only the conceptual model and the numerical model? *Everyone is a model user even if they do not see themselves as one.*

A question arose about what constitutes the "subsurface" in subsurface contamination. It could be defined as being from the ground surface to different depths, or it could depend on the scale of the problem. We have data from other sites to make a first cut of a model. Site data can be used as it becomes available. The essence of modeling is to use data from other sites, and update the model as additional knowledge becomes available. The issues involved in undertaking modeling need to be clearly defined.

Other questions involve regulatory fiction (where regulators tell the modeler to leave out existing cover in the study), and conservative versus realistic approaches. The appropriate level of detail to include in a model needs to be identified. This may drive people to look at more complex processes when they are not warranted. If the model is misapplied, the conceptual model is not correct. There is a need to challenge the assumptions in the conceptual model.

A question was posed to participants from Russia as to whether there is a conflict between the cleanup process and onlookers? Environmental impact statements are prepared by scientists, and the applicants want to justify their position based on modeling. An independent review will be done with some public involvement. For example, there was recently a year-long discussion on building a nuclear power plant in the southern Urals. In addition to the environmental impact statement, there was a large-scale effort to get the public involved and in favor of the project. Everyone was happy with the feasibility study. The safety analysis report showed that the plant could be built safely. Both the scientific community and the public were convinced. Regulatory oversight included a review of drinking water quality. When drinking water reserves are assessed, the qualitative and quantitative findings are taken into account. The feasibility of safe operation on water quality is not made by the public, but by an expert independent panel. The expert panel (appointed by the state commission on the environment) does a complete overview.

3. What is the size/imminence of this problem?

4. What is the current level of effort toward solving the problem(s)? When is enough?

Discussion: Is dose to a receptor based on a well-characterized source? Do social, political, and economic factors enter the modeling? These factors do affect the acceptable dose limit. Problems concerning radioactive waste include decommissioning, low-level waste, and high-level waste. Possible doses go from low to high. Areal extents go from low to high. The time frame goes from short term (100 years) to long term (thousands of years or more). We are looking at events ranging from the likely to the possibly rare. Modeling difficulty ranges from easiest to hardest. Decommissioning is real time, so it is possible to see if your results are correct. The process can be made even harder because of the scrutiny.

Models that can be used for decommissioning now include a screening model. This has the least expensive site-specific information, but may over estimate dose. A high-level model is more expensive. Ideally, a usable model should be available now, with user manual documentation and verified results, but no such model is available today.

If we compared two identical sites, one in Russia and the other in the U.S., would two scientists using the same model get the same result? (They should, but for WIPP, the model development and models were driven by public perception of the waste stream.) Long-term predictions such as radioactive waste disposal are based on little data, long time scales etc. The subjectivity makes the modeling difficult. We need to evaluate how to get the correct results applicable to the physics of the site. Only then do we have to investigate the other factors (e.g., political, social, economic) that relate to the problem. Provided the model is correct for the modeling of a physical phenomena, there is only one possible result. The only thing arguable is the uncertainty of the result. (For WIPP, the conceptual model development was driven by assumptions that the stakeholders made concerning the site. The real world does not make clean distinctions between the scientific model and the social model. Many modeling exercises are schedule driven, and the technical community may apply different models for the same question depending on the time allotted for the modeling exercise.) There are conceptual, mathematical, and numerical models. Once the conceptual model is defined to the satisfaction of everyone concerned, two modelers should get the same result. The conceptual model contains the social, political, etc., concerns.

Another important use of modeling is assessing alternative remediation strategies. The economic factor clearly affects the modeling. DNAPL models may need to be developed.

5. Have modeling, simulation, and analysis been used to address problems in this interest area, and if so, which ones and how effectively?

Discussion: Models used extensively for these types of problems include predictive models, inverse models, specialized models (e.g., geostatistical models), deterministic versus uncertainty, and detailed process models against integrated system models. System models are deterministic, with uncertainty coming from our lack of understanding. It is troubling to some that there is no way to reduce uncertainty, but the spending effort is on models that handle the uncertainty. We need to have the uncertainty analysis. The best use of uncertainty is to decide where next to gather data, locate a well, etc. We also can make a sound decision to stop gathering data based on uncertainty.

6. What can be done with modeling, simulation, and analysis in this area? (Examples, success or non-success stories)

7. If modeling and simulation is not being used, or not being used successfully, why not?

Discussion: There is no information on models that handle the interaction of radionuclides with rock (geo-chemistry, sorption/desorption, diffusion). At some sites, the stakeholders do not want modeling. The site is just cleaned up (e.g., the soil is removed). Politics may drive site cleanup.

Modelers have not communicated results effectively to decision makers. The general population does not understand the technical community. Even science education within the school system does not provide the basis for understanding modeling. At the same time, many modelers have unrealistic expectations and credibility problems. What is needed is a prediction to see if the site needs to be cleaned, and an analysis as to whether the problem will be made worse by cleaning the site up. The total picture is not known unless you model the site. We have developed a number of models, but they cannot incorporate everything. There is never enough data. We will never be able to access natural phenomena in its totality. In Russia, their site model has been continuously improved. They have been using this process for over 30 years, and continuously use feedback to update the models and the results.

8. Is there a gap between the development of models and simulation tools and methodologies and their application? Are new models, tools, and/or methodologies needed?

Discussion: There are impediments to using models to make decisions. Because of certain pressures on models (e.g., tight schedules, limited resources, communication gaps) models are not always ideal. The best way to work effectively with decision makers is to educate them in advance, support them in real time, and analyze the fallout. Constant educational effort is required. Marketing and advertising about modeling achievements may be needed. This may be because modelers oversell their wares or maybe just because there are so many different viewpoints/ backgrounds. Expectations are too high, leading to frustration. We need to recognize that models have limitations. An example of a case in Russia where communication was established very quickly concerned a power plant. By quickly modeling a problem that was of interest to the power-plant managers on a particular day, they readily accepted a longer-term emergency response plan. When the objectives are clear, the customer is usually satisfied. Sometimes the modeler is not up to the task, and the product is not adequate. Modelers should document why a particular method or model was used for a process.

There is a need for off-the-shelf, reliable models. Modelers cannot develop everything, and they need to know when they have done enough. Interdisciplinary teams and team feedback are very important for this purpose. Modeling is best used as an iterative process with data collection. Sometimes this is not feasible because of the objectives of the managers, the schedule etc.

Areas in which there are gaps between the development of models and their applications are as follows:

a. Reactive Chemical Transport. Models with sophisticated flow and transport or sophisticated geochemistry exist, but they are not combined into a single code. We are nowhere near being able to deal with natural systems. Scaling is a big issue: Do we need to develop effective models that do not have the full-blown geochemical reactions, but possible mass transfer limitations? We need models that are computable. Even a single column study with complicated geochemistry cannot successfully be modeled. What extent of accuracy should we strive to achieve in modeling these sorts of processes? Models have to be based on data. For example, in acid mine drainage, you need the true chemical processes to understand the problem. The data gathering effort needs to provide the modeler with the data; otherwise, the objective cannot be met.

Chemical processes lead to continuous changes. For example, Kd for Sr can be measured in the lab, but in natural conditions, it may not apply. The utility of lab data is in question for the field scale. There is also a need for new fundamental chemical and mineralogical data, integration of multidisciplinary teams, and computer hardware and software development. The field data must be sufficiently detailed to allow comparison with the detail of the modeling effort. Data collection and the modeling effort are coupled and drive each other.

b. Immiscible Fluid Flow. Fluid instabilities and heterogeneity (fingering) are particularly troublesome for calculating immiscible fluid flow. Also, hysteresis (change in wetting fluid where oil becomes the wetting fluid rather than water), the partitioning between gas and liquid phases, is also troublesome. At a larger scale, we cannot assume equilibrium. We may need a mass transfer model. This is a scale issue.

c. Hardware/Software. Discretizing space and time leads to numerical dispersion. We need numerical dispersion, interdisciplinary teams, and robustness of solvers.

d. Scaling Heterogeneity. Scaling is especially severe with respect to reactive chemistry, biological models, and phase transitions. Different scaling issues include pore-scale to large-scale and detailed process models to site model.

e. Biological. We will never be able to model all the microbial activity in a large-scale system, so we need to understand the small scale in order to understand what is not being included in the larger-scale model. Very small-scale processes can drive the system. The problems listed above for reactive chemical transport also apply to the biological. Microbes are everywhere, appearing in laboratory experiments and field sites. The vocabulary of microbiologists is very different from hydrologists. Biology is a hard multidisciplinary task. Sustained multidisciplinary effort by DOE on this subject is suggested. Models of this type have become important because predictive results sometimes do not match the data.

f. Colloid Transport.

g. Uncertainty. If we are unable to predict and identify where the gray areas are, our credibility is eroded. Our ability to calibrate the model to the data is poor, and calibration efforts are arbitrary. We need better insight. Inverse modeling may help this, but it needs to be applied intelligently. Using multiple types of constraints is an artistic method. A more rigorous methodology is needed. At Golder, Basian probability is used. This provides a balance between basic scientific ideas, data in the field, and general knowledge of data and processes gained from other sites/history (e.g., shale from another site). A balance of these three elements is needed for the calibration. It is difficult to convey uncertainty to senior decision makers. We tend to make do with the data that we have, rather than making plans to collect data that would be useful. Integrating risk analysis models is desirable.

h. Hydro Mechanical Process Models.

9. Have there been cost/benefit studies for various models and simulation, and analysis tools and methodologies? Do we expect a good payoff if efforts are expanded into modeling and simulation?

Discussion: A cost-benefit analysis is essential. Modelers cannot model without knowing their objectives. This may not have been an option in the past because of the lack of modelers and of models to do this. Now we can compare remediation technologies and use this information for site characterization to lead data gathering efforts. A huge cost benefit can result, as in the case of WIPP. A predictive model can be used to determine the more economic remediation strategy.

There must be a cost-benefit reason to even do model development. The cost benefit of using a model versus not using a model could be discussed in a qualitative manner. Modeling is just one tool in achieving these objectives. The cost of model development is insignificant compared to the questions that it can answer. Modeling should prove the economic benefits of our approach. We either march ahead in darkness or use the models to light the end of the tunnel. With today's state-of-the-art computers, costs become less. At the Savannah River site, new technologies (OTD) include a cost-benefit analysis. Permitting, monitoring, and acceptability are all included. Cost comparisons are made of different strategies at the same site.

Decision makers in EM are not convinced that modeling is useful to them. Disagreement among modelers does not reflect well to the regulators. Formation of a few teams to show and educate the regulators could help alleviate this problem. Also, it may be helpful to do a cost-benefit analysis after the fact at some sites that have and have not used models to determine whether there were benefits in modeling the site. A comparison of modeling versus no modeling would show the benefits derived from modeling. It may be beneficial to EPA to do a cost-benefit of using a sophisticated model versus a simple model. The degree of modeling should be proportional to the degree of the problem. More needs to happen in this area.

Have any criteria been established to perform a cost/benefit analysis? To sell modeling to decision makers, a cost-benefit approach may be the best way to go. If we put this issue on the table, red tape may prevent there being any money for simulations. Many modeling studies can be matched with a calculator and a back of the envelope calculation. The perception is that the more complicated model provides the better answer.

Consensus may be as important as predication. Developing the model and inserting parameters into it gives insight into the problem. Modeling gives insight, not true answers. The incremental benefit of using two-dimensional versus three-dimensional models is seldom considered. Decision analysis at WIPP is using models to help save money. Models should be used to look at the whole system. Integrated systems is the goal.

Desktop computers have lowered modeling costs compared with the old, expensive Crays. We can start with inexpensive models to look at the components of the system and then combine the parts into the system models. Modeling costs almost nothing compared to other costs, but the benefits are tremendous. Again, while the cost of modeling may be low, the cost will seem high if the model’s limitations are not well understood and the modeling effort is oversold.

10. What modeling and simulation techniques are shared with other interest groups?

Discussion: Techniques are shared with the Health and Ecological Effects, Environmental Security, Actinides, and Manufacturing/Pollution Prevention interest areas.

11. What are the other benefits that can be obtained from modeling and simulation?

Discussion: The team discussed modeling versus not modeling and some examples of large-scale ponded field tests and measuring of Sr were given. There is a need to look at analog sites and to design experiments by looking in the right place. The synthesis process can show whether you understand your system or not. Modeling is used for test design and monitoring. You should modify a test design until you get the kind of sensitivity you need. For example, during one field experiment, the ability to measure the flow rate was lost. Afterward, models were used to calculate the flow rate based on measured data, and the field experiment was successful.

Models assist in setting operating parameters. In addition to the economic benefits, another benefit is the optimization and update of the operating procedures (reverse engineering). This is a complicated process. Sometimes we cannot always trace back all the way through the process, but feedback from modeling gives us a better understanding. This might be more important than the economic benefits. For example, in one experiment the initial data from some of the distribution factors was changed as new data became available. From an operating point of view, the experimenters were able to determine which wells should be put online. The operator always addresses the model.

A model can tell you when enough is enough, when to stop data collection, when to stop monitoring, when to close the site, etc. A model produces results in better than real time. A modeling exercise can be repeated under different sets of conditions, and different scenarios can be evaluated. The modeler should model extreme conditions—the "What ifs?" Airline pilots fly simulators for this same reason. Experimental programs are threatened when the experimenter says that some data may not be needed (or that some programs may be needed.) This is a cost benefit even if it does annoy the experimentalists.

12. What measures can be used for assessing how well modeling, simulation, and analysis are being applied?

Discussion: The team felt that continued funding is not a good measure because some projects receive continued funding even though they are not good studies. Valid measures are:

1. Are your modeling results integrated with the major decision milestones? Are results implemented and used by the customer?
2. Do you have access to (or are your results accessed by) senior decision makers?
3. Will the data collectors talk to you and share their data? There must be interaction between the modelers and the experimentalists.
4. Did the modeling save money?
5. Did it prevent a bad situation?
6. Was there improvement in the conceptual model? (Hypothesis testing, reducing uncertainty.)
7. Did it reduce site characterization costs?

8. Was your work published in a peer review publication? Sometimes when field results are shown to managers, they do not mean much, but when modeling results are shown to managers to help them view the data, it is very effective.

Appendix K. Subsurface Contamination II

Subsurface Contamination II Interest Area Team

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This interest area team addressed the questions that were given to the teams as guidance and discussed at length the benefits of modeling and simulation. The team felt that the full benefits of modeling and simulation (i.e., cost-effective cleanup) in the area of subsurface contamination can be realized only in a systematic framework that relates site activities to clearly defined objectives. These objectives should be developed with the early and continuous involvement of a management team made up of decision makers, site managers, regulators, stakeholders, and modelers (scientists/engineers). In the context of this holistic framework, modeling provides the organizing infrastructure to guide site activities that are responsive to decision making needs.

The team felt that in view of our limited and evolving understanding of contaminant behavior at a given hazardous waste site, our models must necessarily adapt to new and better information that can alter management strategy. Thus, there is an explicit and dynamic linkage between data collection (characterization and monitoring), assessment of remediation options, optimization of remedial design, the management team, and the decisions that need to be made.

Questions and Answers

The team rephrased the questions given as guidance as noted below.

1. What is it that we know how to do well now?
2. Given that, why don't people use it; how can we enhance the use?
3. What do we *not* ***know how to do well?***
4. How can we justify further research when present capabilities are not being used or not being fully used?

Discussion: Modeling is used in characterization (geology, hydrology). There are a number of things we do well, such as in the areas of standard saturated flow and simple transport in aquifers. Codes can run very high resolution, but data at high resolution is not available. Given this, how well do we include that uncertainty/lack of data in our models? This is an area of development. What are traditional approaches and their weaknesses? MODFLOW and MT3D are widely used. GUI/GIS interfaces are used.

· Saturated flow—solute transport-simple geochemistry. Conservation laws are well established, but constitutive relations are where things can get complicated and site specific. Do we know how to deal with hydrocarbons (e.g., TCE)? We can do fairly well for many solutes that behave linearly, or approximately linear.

· Unsaturated flow—single phase. User friendly tools exist, but their use is not necessarily straightforward (calibration, sensitivity, formal repeatability). Classes of uncertainty include geologic and properties, parameterization, and numerical. The more heterogeneous the site, the less certain; even the simple cases are not done as well. Dispersion is a complicating factor, as well as fractures.

· Unsaturated zone—We should be skeptical of codes being used that are not specifically designed for the application. Technology is there, but greater care is needed in its application. More experimental validation is needed. Saturated zone chemical coefficients cannot be directly carried over.

· Remediation—What are state-of-practice remediation methods?

- grid resolution usually too low
- pump and treat and optimized pump and treat
- hydraulic barriers/barriers
- natural attenuation (e.g., TCE) aerobic
- soil vapor extraction
- air sparging

· Characterization from limited data—trial and error and inverse techniques. We are better at comparisons than at absolute magnitudes. For complex geology, gridding is important. Off-the-shelf applications are not available. State-of-practice modeling is generally what we do well. Two-dimensional is frequently used. Modeling detail should be commensurate with modeling objectives and data available. We need to articulate the relative applicability of models/codes. Codes are available to simulate the remediation methods listed above.

· Stochastic modeling—This includes Monte Carlo, moment analysis, perturbations, kriging (geostatistics-conditional simulation-spatial variability), turning bands (for Monte Carlo), and parameter estimation techniques. There are limiting assumptions such as stationarity, small perturbations. Stochastic methods are not widely used partly because of a lack of education on the part of potential users. In an accurate computation of pressure head versus velocities, the first is easy, the second is more difficult.

· Fully saturated transport

- kinetics versus simpler Kd approach
- radionuclide transport
- reactive transport (metals, speciation, redox, organics, coupling of inorganic and organics, density dependent on concentration). Issues include a lack of thermodynamic data; temperature effects; field scale verification of these kinds of models; and accessibility and training. In addition, they are more difficult to use and require more expertise.
- fractured systems
- microbial reactions
- knowledge gap; research item: scale-up of permeability and dispersitivity (e.g., Gelhar model seems to be useful for some sites).

· Variably saturated (Richards equation)—Research items include ET (evapotranspiration), barometric pumping, recharge; water-dependent anisotropy; hysteresis; soil-water curves; arguments about whether these are state of the art or R&D categories (e.g., hysteretic models have been applied to field data successfully); and coupling of surface flow and subsurface flow.

· Transport—solutes; vapor phase diffusion; isothermal, nonisothermal; geochemistry.

· Multi-phase flow—two-phase; NAPL issues (for lower NAPL saturations, constitutive relationships are not well known); multicomponent issues (need good GUI/GIS for user-friendly mode; three phase relationships, wettability concept; adaptive gridding (AMR); interface transfer; optimization (has not been applied to many situations); remediation (bioremediation); nonisothermal.

5. What is the value-added of going to state-of-art from state-of-practice?

Discussion: Value added includes better accuracy and efficiency and increased confidence. We know better how uncertainties are related to measurements. There is the value of bringing over technology from other disciplines (e.g., oil and gas). Added value will vary from site to site (easy, standard, versus complex). Are there any documented examples? Monitoring, ability of innovative technology to compare various options-cost comparisons, risk comparison, source term, delineation. Web sites include Mound (Sandia), the LBNL web site, and the LLNL web. Issues include cost comparisons, O/M capital costs, data collection/monitoring. Other value added issues include regulator acceptance; “what if” scenarios;

probability of failure; leadership in problem solving; effective use of data and data management; problem solving environments, and integrated framework.

What is the value of modeling for WIPP and Yucca Mountain? (Regulatory compliance issue; also to provide some level of confidence.)

6. *Does modeling require more site data than would be needed if modeling was not used?*

Discussion: It might if you are only interested in capture zone analysis. However, the manager should realize that even in simple situations he/she is in effect creating a mental model of a site and processes operating. Same data used to create a conceptual model is the same that would be needed to create a numerical model. If you have enough data to create a conceptual model, you have enough to run a simulation. How much data is "enough"? Modeling should be incorporated from the beginning, to help with the design of data sampling. This is even more important for innovative remediation methods. Regulators seem to be more aware of value of modeling than managers; they want a documented model with a well-founded basis. Managers often have the attitude that it is easier to spend money later rather than now. There are new algorithms to formally optimize the location of data sampling, or remediation efficiency, either "all at once," or on the fly (e.g., using sampling of a migrating plume to indicate where to put the next well to reduce uncertainty). Monitoring and modeling should go hand in hand. Team work is important. One can progress from simple modeling to more complex modeling at a site (e.g., take some measurements, strategically placed). Based on the results of modeling using that information, monitoring can be extended. Modeling can sort out which processes and factors are most important for success of in situ innovative technology, which will give some indication of which types of sites are good candidates for the technology. Legal problems might result if you cannot show that the modeling that is done is standard practice. Some financial incentive should be provided to contractors to spend dollars on innovative ideas for modeling.

7. *What are impediments to more effective use of modeling?*

Discussion: Impediments include:

- Communication and trust with public
- Visualization pros/cons
- Modelers tend to emphasize the model as an end in itself
- More independent peer review is needed
- Negative perception on the side of the public and managers because of past abuses, failures, and expectations that were too high
- Failure to involve regulators from the beginning of the effort

8. *How can we market ourselves more effectively?*

Discussion: Communication with regulators and the public, and mutual education of regulators and the public, is vital. Managers need to be educated to speak both languages (technese and managerese). We need to integrate modeling into our changing culture. Sometimes, it is difficult to find the group that has authority to institute changes to promote new technology. Getting to high level management would be most effective. Another big impediment is the fear of failure. If managers think the risk of failure is low, they are often more receptive. We can learn from other disciplines/areas (e.g., the oil industry). The oil industry spends big dollars to support and advance modeling and to promote communication between modelers and non-modelers in the business. DOE STCG technology needs are not filtering down to the modeling community. There is a big disconnect between headquarters and the modeling community, as well as a lack of communication among government agencies.

Other discussions regarding effective marketing included the issues of decision support, strategies, and simulation/optimization levels (e.g., joint analysis). In the area of decision support, the team discussed optimization and simulation, economics, time/costs, and performance criteria. In the area of strategies, the team discussed ecological impacts as well as health and uncertainty/sensitivity. In the area of simulation/optimization levels, the team discussed public/regulator/stakeholder involvement, social constraints/subjectivity, adaptive management, and the need for an integrated framework—the integration of all the above into one system. The team also discussed the timeline effect of today on tomorrow (e.g., the 30-50 year time frame and the implicit expectation that a site will be cleaned up within that time interval), the export and portability of results, ties to business practices, and multimedia risk assessment.

9. What results do we need to show to a decision maker?

Discussion: Results might include a cost-risk plot and simulations (e.g., 3-D flow fields, plume). We need to know what help decision makers need as opposed to what we think they want or need.

10. What do we need from decision makers?

Discussion: Communication of what management and decision makers need is essential, and modelers should be involved in the decision-making process. We should encourage investments in demonstrations that show the advantages of new technology. This could include site demonstrations, incentives, an integrated/partnered framework, a larger program of planned involvement, and a holistic approach to modeling. We need a cradle-to-grave perspective.

Recommendations

The Subsurface Contamination II interest area team proposed the following recommendations and conclusions:

(1) ***Improve Communication.*** The information exchange between modelers, regulators, decisionmakers, and stakeholders is critical to successful remediation. The team recommended setting and meeting the following goals:

- Establish clear objectives and expectations.
- Communicate the objectives and expectations early and often.

- Communicate technical information in a form suitable to decisionmakers (e.g., risk versus cost).

(2) ***Improve Integration of Cleanup Activities.*** Non-integrated cleanup activities incur additional cost and risk. The team recommended that cleanup activities be integrated. The following should be done to ensure that necessary activities *are* performed while unnecessary activities are *not*:

- Establish a clear link between each activity and its correlated decision making process.
- Establish a mechanism, such as a database, to adapt to new information.
- Use the best available technology.

(3) ***Adopt an Holistic Approach to Remediation Projects.*** Focus on integration, not just organization. The team recommended setting and meeting the following goals:

- Establish a systematic framework that truly integrates the project activities in support of the decision making process.
- Formulate work teams that include at least one modeler, one field scientist, one manager, one regulator, and one stakeholder.
- Ensure that management teams communicate (not just inform) early and often.
- Implement modeling tools that link project activities by using a mechanistic understanding of contaminant behavior in environmental systems.
- Implement an adaptive management infrastructure.

(4) ***Provide Incentives for Using the Best Available Remediation/Modeling Technology.*** Providing such incentives will promote excellence over parochialism. The team recommended setting and meeting the following goals:

- Insist on realistic lifecycle costs when assessing technologies.
- Reward the deployment of demonstrated innovative technologies.
- Provide opportunities to demonstrate the benefits of the integrated project framework described above.
- Reward the use of advanced simulation capabilities that improve the resolution of process mechanisms important to the remediation.
- Provide opportunities to demonstrate the benefits of advanced computational (e.g., algorithmic and computer science) and mathematical (e.g., optimization, probabilistic) approaches that improve decisionmaking and project management/ business practices.
- Reward partnering between government agencies.

Appendix L. Waste Treatment

Waste Treatment Interest Area Team

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The Waste Treatment interest area team began its discussions by considering the major problems in process modeling and simulation. It was noted that (1) most efforts and modeling/simulation problems were site-specific with little effort and incentive to make them more generic in nature; (2) little effort is made to evaluate when data gathering becomes excessive or of diminishing value; (3) too little effort is made to model treatment processes when the database available has a broad band; and (4) not enough effort is made to improve data management and reliability. Modelers should do more to include uncertainty in their models. Modelers should also include more coverage of downstream effects in their system (e.g., build in a more generic effect). While these were the major overview process problems discussed, several minor problems surfaced: for example, how do we model public acceptance? How do we better communicate with decision makers? How do we express a higher level of comfort and reliability to the decision makers in regard to modeling and simulation?

Important Needs

The team re-evaluated the generic problems discussed above in order to develop more specific suggestions of needs. The four greatest needs identified by the team were as follows:

(1) A fully integrated system for waste treatment is needed that includes, at the very least, a consideration of life-cycle effects, waste quantity, the risks presented by the wastes, and waste transport.

(2) DOE Complex-wide generic models need to be developed and applied at each site. The team felt strongly about this, and also felt that new technologies or competing technologies should be evaluated as modeled systems. The models should include costs, waste forms, classification of waste (e.g., TRU-waste, low level), environmental impacts, risks, and safety measures. Other potential areas that need to be modeled that were discussed by the team included (in approximate order of priority) the use of uncertain data; projected waste loads; project schedules; treatment optimization; long term storage models; safety rules and guidelines; availability of technology;

technology reliability; no-action scenarios; socio-economic issues; air pollution control on treatment processes; and optimization of business practices.

(3) Advantages of modeling and simulation in waste treatment systems include such little recognized needs as improving the institutional memory of treatment methods and systems. Models would identify, through sensitivity analysis, what is more important and where the critical paths are, and aid in the communication of these findings. Models should aid decision makers in understanding where the particular problems are, and greatly enhance their knowledge and understanding of waste treatment problems in general. Other important advantages of online models are that they save money, reduce risk, reduce waste, and point the way to improved design changes.

(4) Metrics are available and should be used to estimate the effectiveness of modeling efforts. These metrics include frequency of use; costs of the model; adaptability to new problems; diversity of use; and supportiveness. A model should be user friendly, well documented, reliable, portable, well defined, and low maintenance. Training in its use must be available.

The team listed several very successful models currently in use, including manufacturing models for the design of protective glass in glove boxes. Each use requires minimum protection standards; without design models for glove box use, special manufacturing models for each window would be required. With proper models, manufacturers can cast glass covers for generic ranges of use at large cost savings. Another example of successful models in use include transportation models used for scheduling and delivery. Such models are in use by large shippers as well as by DOE for depository scheduling.

Many treatment processes have been modeled. Routine site modeling is now performed with pollutant transport functions. Failure mode characterization is performed by models for various materials in widespread use, and practically all risk estimates are performed with modeling and simulation. Why then is modeling and simulation not being used more widely? The most frequently cited reasons are data uncertainty or data unavailability, but a truer reason may be the lack of an adequate definition of the model and data needs. A major problem is the lack of available time and financial support. The lack of incentive to integrate existing models to other sites for use is yet another issue.

Managers do not fully appreciate, and modelers do not clearly communicate, the useful nature of model outputs. The frequent lack of site specificity in generic models is also cited as an impediment. The need to identify and integrate (link) existing models is great, but to do so requires a tremendous amount of advance planning for validation and integration. A major impediment is the general lack of a built-in system to allow integration from site-specific models to more generic ones. None of the team members offered any evidence or knowledge of cost/benefit studies done on modeling and simulation, but all participants felt these studies were essential.

Recommendations

The two basic recommendations of the team were to:

(1) Integrate and expand site-specific models to DOE Complex-wide application models.

(2) Create a DOE Complex-wide Council on Modeling and Simulation—an incentive to make use of existing models that work well rather than inventing them. Many good models exist that are only applied to limited efforts.

The Council on Modeling and Simulation could be patterned on the Strategic Laboratory Council, with a representative from each laboratory, a representative from each major site, and representatives from major contractors. For a reasonable resource investment, the best of the Complex could be set to work on integration of waste treatment problems.